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# A Priori Error Analysis of Two Force-Based Atomistic/Continuum Models of a Periodic Chain

Charalambos Makridakis · Christoph  
Ortner · Endre Süli

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**Abstract** The force-based quasicontinuum (QCF) approximation is a non-conservative atomistic/continuum hybrid model for the simulation of defects in crystals. We present an a priori error analysis of the QCF method, applied to a one-dimensional periodic chain, that is valid for an arbitrary interaction range, large deformations, and takes coarse-graining into account. Our main tool in this analysis is a new concept of atomistic stress.

Moreover, we formulate a new atomistic/continuum coupling mechanism based on coupling stresses instead of forces and extend the a priori analysis to this new method. We show that the new method has several theoretical advantages over the original QCF method.

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C. Makridakis

Department of Applied Mathematics, University of Crete, GR 714 09 Heraklion-Crete

Tel.: +30 2810 393726

Fax: +30-2810-393701

E-mail: makr@tem.uoc.gr

C. Ortner

Mathematical Institute, University of Oxford, Oxford OX1 3LB, UK

Tel.: +44 1865 615106

Fax.: +44 (0)1865 273583

E-mail: ortner@maths.ox.ac.uk

E. Süli

Mathematical Institute, University of Oxford, Oxford OX1 3LB, UK

Tel.: +44 1865 273525

Fax.: +44 (0)1865 273583

E-mail: sul@maths.ox.ac.uk

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## 1 Introduction

Atomistic/continuum hybrid models are often employed to describe localized defects in a long-range elastic field. While atomistic models are needed to provide accurate descriptions of defects they are usually too expensive computationally to allow sufficiently large-scale simulations that resolve the elastic far-field, which can, instead, be modelled efficiently by a coarse-grained continuum model. Methodologies for coupling the two different material descriptions were first described in [16, 15, 24, 31]; more recent examples are [1, 11, 32, 14, 28]. The numerical analysis of atomistic/continuum hybrid methods is a topic of active research [4, 5, 8, 9, 11, 12, 17–19, 23, 25, 26]. We also mention [22, 21] for recent overviews of the field.

Despite several creative (and sometimes complex) attempts [11, 30, 32] considerable obstacles remain for the formulation of accurate *energy-based* coupling mechanisms. By contrast, *force-based* coupling mechanisms [4, 16, 15, 31] are comparatively simple in their formulation and, more importantly, they do not suffer from the interfacial consistency errors exhibited by most energy-based methods [5, 23]. The force-based quasicontinuum (QCF) method [4] is a prototypical example of a force-based atomistic/continuum hybrid method and is the focus of the present paper.

A series of recent articles [7–10] was devoted to the study of a linearized QCF operator in one dimension. This analysis revealed some unexpected and potentially undesirable (in)stability properties. The fact that the QCF method makes no modification of the forces at the interface gives rise to a hidden coupling mechanism that can only be observed in a weak representation of the operator and has the effect that the QCF operator is generically indefinite and that it is unstable in discrete variants of  $W^{1,p}$ -spaces for  $1 \leq p < \infty$ . Nevertheless, it is possible to prove stability in a discrete  $W^{1,\infty}$ -space [9], a fact we shall also use in our error analysis.

The first purpose of the present work is to extend the analysis of the QCF method to include finite range interaction, large deformations, and also to take into account the coarse-graining of the continuum model, a step that was previously disregarded. Our analysis is still restricted to a one-dimensional model, which is primarily due to the fact that we are lacking the techniques that would allow us to prove stability in higher dimensions. Our main tools in this analysis are a new atomistic stress function (Section 3.1) and the resulting atomistic/continuum model error estimate in terms of stresses (Section 3.2). Moreover, the atomistic stress function provides a new perspective on the interface terms in the weak form of the QCF operator (Section 4.1). In Sections 4.2 and 4.3 we establish stability and consistency of the method in a suitable function space setting, which we combine into an a priori error estimate in

Section 4.4. We obtain a superconvergence result that is formally of second order.

The second purpose of this paper is to formulate and analyze a new force-based coupling mechanism that does not suffer from the deficiencies of the QCF method mentioned above. Our starting point is the observation that the stress is a more natural concept in continuum mechanics than the force. Indeed, since we have a representation of the atomistic force in its weak form in terms of the atomistic stress function it is natural to couple stresses as opposed to forces (as in the QCF method). This leads to a new stress-based atomistic/continuum coupling mechanism (SAC method) that we analyze in Section 5. Our results for the SAC method are similar to those for the QCF method except that they are valid in a larger deformation regime. Moreover, we show in [20] that the SAC operator is positive definite, which might make an extension of the error analysis to two and three dimensions feasible.

To conclude we present in Section 6 several numerical experiments confirming our analytical results.

## 2 Formulation of the QCF Method

### 2.1 Notation for discrete functions

We begin by briefly introducing some notation for discrete functions. We shall be concerned with functions defined on  $\mathbb{Z}$ , which we shall denote by  $v = (v_\xi)_{\xi \in \mathbb{Z}} \in \mathbb{R}^{\mathbb{Z}}$ . Of particular interest are periodic functions with a period  $2N$  where  $N \in \mathbb{N}$ ,  $N \geq 2$ , is fixed throughout. The set of  $2N$  periodic functions is denoted by  $\mathbb{R}_{\#}^{\mathbb{Z}}$ . We define the reference cell as

$$\mathcal{L} = \{-N+1, \dots, N\}.$$

Throughout, we set  $\varepsilon = 1/N$ .

For  $\mathcal{K} \subset \mathbb{Z}$  and  $p \in [1, \infty)$  we define the (semi-)norms, for  $v \in \mathbb{R}^{\mathbb{Z}}$ ,

$$\|v\|_{\ell_\varepsilon^p(\mathcal{K})} = \left( \varepsilon \sum_{\xi \in \mathcal{K}} |v_\xi|^p \right)^{1/p}, \quad \text{and} \quad \|v\|_{\ell_\varepsilon^\infty(\mathcal{K})} = \|v\|_{\ell^\infty(\mathcal{K})} = \max_{\xi \in \mathcal{K}} |v_\xi|.$$

Whenever the set  $(\mathcal{K})$  is omitted from this notation, then it is assumed that  $\mathcal{K} = \mathcal{L}$ . For  $p = 2$  and  $\mathcal{K} = \mathcal{L}$  the associated inner product is

$$(v, w)_\varepsilon = \varepsilon \sum_{\xi \in \mathcal{L}} v_\xi w_\xi \quad \text{for } v, w \in \mathbb{R}^{\mathbb{Z}}.$$

Using the convention  $1 = (1)_{\xi \in \mathbb{Z}}$ , the set of periodic functions with mean zero is denoted by

$$\mathcal{U} = \{v \in \mathbb{R}_{\#}^{\mathbb{Z}} : (v, 1)_\varepsilon = 0\}. \quad (1)$$

For  $v \in \mathbb{R}^{\mathbb{Z}}$  we define  $v' = (v'_\xi)_{\xi \in \mathbb{Z}}$  and  $v'' = (v''_\xi)_{\xi \in \mathbb{Z}}$ , where  $v'_\xi$  denotes the backward finite difference and  $v''_\xi$  the centered second difference,

$$v'_\xi = \frac{v_\xi - v_{\xi-1}}{\varepsilon}, \quad \text{and} \quad v''_\xi = \frac{v_{\xi+1} - 2v_\xi + v_{\xi-1}}{\varepsilon^2}.$$

(Note that with this notation  $v'' \neq (v')'$ .) The first-order discrete Sobolev norms are defined as

$$\|v\|_{\mathcal{W}^{1,p}} = \|v'\|_{\ell_\varepsilon^p} \quad \text{for } v \in \mathbb{R}^{\mathbb{Z}} \quad \text{and for } p \in [1, \infty].$$

We note that  $\|\cdot\|_{\ell_\varepsilon^p}$  and  $\|\cdot\|_{\mathcal{W}^{1,p}}$  are norms on the space  $\mathcal{U}$ .

Finally, we adopt the convention that all functions  $v \in \mathbb{R}^{\mathbb{Z}}$  are identified with their continuous piecewise affine interpolants with respect to the reference lattice

$$x = (x_\xi)_{\xi \in \mathbb{Z}} = (\varepsilon \xi)_{\xi \in \mathbb{Z}}.$$

With this convention we have, for  $v \in \mathbb{R}^{\mathbb{Z}}$  and  $\xi \in \mathbb{Z}$ , that  $v_\xi = v(x_\xi)$  and  $v'_\xi = v'(s)$  for  $s \in (x_{\xi-1}, x_\xi)$ .

## 2.2 Atomistic model problem

In order to avoid the complications associated with relaxation effects in boundary layers [26], or the analytical difficulties in infinite domains, we pose an atomistic model problem in a periodic domain. Recalling from (1) the definition of  $\mathcal{U}$ , which we henceforth call the *displacement space*, we define the set of admissible deformations as

$$\mathcal{Y} = \{y \in \mathbb{R}^{\mathbb{Z}} : y - Ax \in \mathcal{U} \text{ and } y'_\xi > 0 \text{ for all } \xi \in \mathbb{Z}\}. \quad (2)$$

The constant  $A > 0$  can be thought of as a macroscopic strain. Thus, admissible deformations are orientation-preserving periodic displacements, with zero mean, from the homogeneous lattice  $Ax$ . We have restricted the set of deformations to functions with positive gradient since the energy functional we are about to define only takes arguments with this property.

We assume that each atom interacts with at most  $r_{\text{cut}} \in \mathbb{N}$  atoms to its left and right, through a pair potential  $\phi \in C^3(0, +\infty)$ , where  $\phi^{(j)}$ ,  $j = 0, 1, 2, 3$ , are bounded in any interval  $[\delta, +\infty)$ ,  $\delta > 0$ . We do not need to assume the typical convex-concave structure of Lennard–Jones-type potentials in our analysis. The *internal stored energy* (per period) of a deformation  $y \in \mathcal{Y}$  is given by

$$\Phi^a(y) = \varepsilon \sum_{\xi \in \mathcal{L}} \frac{1}{2} \sum_{r=\pm 1}^{\pm r_{\text{cut}}} \phi(|D_r y_\xi|), \quad \text{where } D_r y_\xi = \frac{y_{\xi+r} - y_\xi}{\varepsilon}.$$

Here, and throughout, we understand  $\sum_{r=\pm 1}^{\pm r_{\text{cut}}}$  as the sum from  $r = -r_{\text{cut}}$  to  $r_{\text{cut}}$ , excluding  $r = 0$ .

Assuming that all external forces are dead loads (i.e., they do not depend on the deformation), collected into a function  $g \in \mathcal{U}$ , the *total energy* is given by

$$\Phi_{\text{tot}}^a(y) = \Phi^a(y) - (g, y)_\varepsilon.$$

The atomistic problem is to find a local minimizer of  $\Phi_{\text{tot}}^a$  in  $\mathcal{Y}$ , that is,

$$\text{Find } y^a \in \operatorname{argmin} \Phi_{\text{tot}}^a(\mathcal{Y}), \quad (3)$$

where “argmin” denotes the set of local minimizers.

*Remark 1* It is often asserted that more general external forces of the form  $g = (g(\xi, y_\xi))_{\xi \in \mathbb{Z}}$ , which could, for example, model a substrate in a Frenkel–Kontorova model, are easily incorporated in the analysis. This is indeed the case when the stability analysis is based on positivity of the linearized operator. However, our stability analysis is based on a technique that makes the extension to these more general external forces non-trivial.  $\square$

### 2.3 The Cauchy–Born approximation

In regions of the domain  $\mathcal{L}$  where the atomistic deformation is regular (in a sense that we will make precise) we may wish to replace the atomistic model by a continuum model. We begin by discussing the case where an atomistic deformation is smooth everywhere. In that case, the model most commonly encountered is the Cauchy–Born approximation. One way to obtain it is to take a fixed deformation  $\bar{y} = Ax + \bar{u}$ , where  $\bar{u} \in C^1(\mathbb{R})$  is 2-periodic and  $\bar{y}' > 0$ , and let  $\bar{y}^{(\varepsilon)} = (\bar{y}(x_\xi))_{\xi \in \mathbb{Z}}$  denote its restriction to the lattice, to obtain

$$\lim_{\varepsilon \rightarrow 0} \Phi^a(\bar{y}^{(\varepsilon)}) = \Phi^c(\bar{y}) := \int_{-1}^1 W(\bar{y}') \, dx,$$

where the Cauchy–Born stored energy function  $W$  is given by

$$W(F) = \sum_{r=1}^{r_{\text{cut}}} \phi(Fr). \quad (4)$$

The proof of this statement is a simple calculus exercise, which we omit. We refer to [2, 13] for more sophisticated justifications of the Cauchy–Born model.

### 2.4 Finite element discretization: the local QC method

To discretize the Cauchy–Born model, we first partition the domain into a finite number of intervals (*elements*). It is often assumed that the nodes of the partition (the shared endpoints of the intervals) are the positions of a subset of atoms in the reference configuration, the so-called *representative atoms* or

*repatoms*. We will make the same assumption here, as it simplifies some aspects of our analysis. The set of repatoms is denoted by

$$\mathcal{L}_{\text{rep}} = \{\xi_1, \dots, \xi_M\} \subset \mathcal{L},$$

where  $0 < M < 2N$  and  $\xi_1 < \xi_2 < \dots < \xi_M$ .

We extend the grid of repatoms periodically, that is, we define  $(\xi_m)_{m \in \mathbb{Z}}$  through the condition  $\xi_{m+M} = \xi_m + 2N$  for all  $m \in \mathbb{Z}$ . We denote the “physical” positions of the repatoms by  $X_m = x_{\xi_m} = \varepsilon \xi_m$ . We define the local mesh size for elements and for nodes, respectively, by

$$h_m = X_m - X_{m-1} \quad \text{and} \quad H_m = \frac{1}{2}(X_{m+1} - X_{m-1}) \quad \text{for } m \in \mathbb{Z}.$$

We denote by  $\mathcal{S}_h^1$  the space of *piecewise linear functions* with respect to the grid  $(X_m)_{m \in \mathbb{Z}}$ . If  $v_h \in \mathcal{S}_h^1$  then we denote its nodal values by  $V_m = v_h(X_m) = v_{h, \xi_m}$ , and its gradient in the interval  $(X_{m-1}, X_m)$  by  $V'_m = (V_m - V_{m-1})/h_m$ , that is,

$$v_{h, \xi} = V_{m-1} + V'_m(x_\xi - X_{m-1}) \quad \text{for } \xi = \xi_{m-1}, \dots, \xi_m.$$

We define the mesh-dependent inner product

$$(v, w)_h = \sum_{m=1}^M H_m v_{\xi_m} w_{\xi_m} \quad \text{for } v, w \in \mathbb{R}^{\mathbb{Z}}.$$

Clearly, the arguments  $v, w$  need not be defined on all of  $\mathbb{R}^{\mathbb{Z}}$ , but only on the repatom grid  $\mathcal{L}_{\text{rep}} = (\xi_m)_{m=1}^M$ . Allowing a slight abuse of notation we will in fact admit any such family  $V = (V_m)_{m=1}^M$ , etc., of nodal values as arguments for  $(\cdot, \cdot)_h$ . For example, we may write  $(v_h, w_h)_h = (V, W)_h$ , and so forth.

Finally, we define the finite element deformation (or, trial) and displacement (or, test) spaces associated with  $\mathcal{V}$  and  $\mathcal{W}$ , respectively, as

$$\begin{aligned} \mathcal{U}_h &= \{u_h \in \mathcal{S}_h^1 \cap \mathbb{R}_{\#}^{\mathbb{Z}} : (u_h, 1)_h = 0\} = \mathcal{U} \cap \mathcal{S}_h^1, \quad \text{and} \\ \mathcal{V}_h &= \{y_h \in \mathcal{S}_h^1 : y_h - Ax \in \mathcal{U}_h \text{ and } y'_{h, \xi} > 0 \text{ for all } \xi \in \mathbb{Z}\} = \mathcal{V} \cap \mathcal{S}_h^1. \end{aligned}$$

For the finite element discretization of the Cauchy–Born model we approximate the potential of the external forces  $(g, y)_\varepsilon$  using the mesh-dependent inner product  $(\cdot, \cdot)_h$ . This gives the total energy functional for the finite element discretization of the Cauchy–Born model,

$$\Phi_{\text{tot}}^c(y_h) = \Phi^c(y_h) - (g, y_h)_h \quad \text{for } y_h \in \mathcal{V}_h.$$

In terms of the vector of nodal values  $Y$  of a function  $y_h \in \mathcal{V}_h$  the functional  $\Phi_{\text{tot}}^c$  can also be written as

$$\Phi_{\text{tot}}^c(y_h) = \sum_{m=1}^M h_m W(Y'_m) - \sum_{m=1}^M H_m g_{\xi_m} Y_m, \quad (5)$$

where  $W$  was defined in (4). We also remark that through our identification of lattice functions with their piecewise affine interpolants the functionals  $\Phi^c$  and  $\Phi_{\text{tot}}^c$  can also be defined on  $\mathcal{U}$ .

The name often given to this P1 finite element discretization of the Cauchy–Born approximation is the *local quasicontinuum (QCL) method*. Hence, in the QCL method, we aim to find a local minimizer of  $\Phi_{\text{tot}}^c$  in  $\mathcal{U}_h$ , that is:

$$\text{Find } y_h^c \in \arg\min \Phi_{\text{tot}}^c(\mathcal{U}_h). \quad (6)$$

## 2.5 The force-based QC Method

Having defined the atomistic model and the local QC method, the definition of the QCF method will be relatively straightforward. Beforehand we briefly discuss the concepts of criticality and forces in the atomistic and continuum model.

If  $y^a$  is a solution of (3) then it satisfies the first-order criticality condition

$$\langle D\Phi_{\text{tot}}^a(y^a), v \rangle = 0 \quad \forall v \in \mathcal{U}, \quad (7)$$

where  $\langle \cdot, \cdot \rangle : \mathcal{U}^* \times \mathcal{U} \rightarrow \mathbb{R}$  denotes the duality pairing between the spaces  $\mathcal{U}^*$  and  $\mathcal{U}$  and the first variation  $D\Phi_{\text{tot}}^a(y^a)$  of  $\Phi_{\text{tot}}^a$  at  $y^a$  is understood to be an element of  $\mathcal{U}^*$  (see Section 2.6.2 for more detail). We call a function  $y^a$  satisfying (7) a critical point of  $\Phi_{\text{tot}}^a$ . Upon defining the *internal atomistic forces*, normalized by the scaling parameter  $\varepsilon$ , as

$$f_\xi^a(y) := -\frac{1}{\varepsilon} \frac{\partial \Phi^a(y)}{\partial y_\xi}, \quad \text{for } \xi \in \mathbb{Z},$$

and collecting them into the vector  $f^a(y) = (f_\xi^a(y))_{\xi \in \mathbb{Z}}$ , the criticality condition can be written more explicitly as

$$(f^a(y) + g, v)_\varepsilon = 0 \quad \forall v \in \mathcal{U}. \quad (8)$$

Similarly, if  $y_h^c \in \mathcal{U}_h$  is a solution of (6) then it satisfies

$$\langle D\Phi_{\text{tot}}^c(y_h^c), v_h \rangle = 0 \quad \forall v_h \in \mathcal{U}_h. \quad (9)$$

We call a point  $y_h^c$  satisfying (9) a critical point of  $\Phi_{\text{tot}}^c$ . In this case,  $\langle \cdot, \cdot \rangle$  also denotes the duality pairing between  $\mathcal{U}_h^*$  and  $\mathcal{U}_h$ . If we define the QCL force vector  $F^c(y_h) = (F_m^c(y_h))_{m \in \mathbb{Z}}$  (note that  $F_m^c$  are generalized forces acting on degrees of freedom  $Y_m$ ,  $m = 1, \dots, M$ ) by

$$F_m^c(y_h) = -\frac{1}{H_m} \frac{\partial \Phi^c(y_h)}{\partial Y_m} \quad \text{for } m \in \mathbb{Z},$$

then the QCL criticality condition (9) is equivalent to

$$(F^c(y_h^c) + g, v_h)_h = 0 \quad \forall v_h \in \mathcal{U}_h. \quad (10)$$



(Recall that arguments of  $(\cdot, \cdot)_h$  only need to be defined on  $\mathcal{L}_{\text{rep}}$ .) We also define the *effective atomistic forces* on the degrees of freedom  $Y_m, m = 1, \dots, M$ , by  $F^a(y_h) = (F_m^a(y_h))_{m=1}^M$ ,

$$F_m^a(y_h) = -\frac{1}{H_m} \frac{\partial \Phi^a(y_h)}{\partial Y_m},$$

and extended periodically for  $m \in \mathbb{Z}$ .

*Remark 2* We note that, if  $\xi_m, \xi_m \pm 1$  belong to  $\mathcal{L}_{\text{rep}}$  then  $F_m^a(y_h) = f_{\xi_m}(y_h)$ . To see this, we first observe that in this case  $H_m = \varepsilon$ . Expanding the partial derivative we obtain

$$F_m^a(y_h) = -\frac{1}{H_m} \frac{\partial \Phi^a(y_h)}{\partial Y_m} = -\frac{1}{\varepsilon} \sum_{\eta \in \mathcal{L}} \frac{\partial \Phi^a(y)}{\partial y_\eta} \Big|_{y=y_h} \frac{\partial y_{h,\eta}}{\partial Y_m} = \sum_{\eta \in \mathcal{L}} f_\eta^a(y_h) \frac{\partial y_{h,\eta}}{\partial Y_m}.$$

If  $\xi_m$  and  $\xi_m \pm 1$  belong to  $\mathcal{L}_{\text{rep}}$  then  $\frac{\partial y_{h,\eta}}{\partial Y_m} = 0$  for  $\eta \neq \xi$  and  $\frac{\partial y_{h,\eta}}{\partial Y_m} = 1$  if  $\eta = \xi$ , which shows that  $F_m^a(y_h) = f_{\xi_m}(y_h)$  is indeed true in this case.  $\square$

To construct the QCF method, we partition the set of repatoms  $\mathcal{L}_{\text{rep}} = \mathcal{L}_a \cup \mathcal{L}_c$  into the degrees of freedom for which we require atomistic accuracy,  $\mathcal{L}_a$ , and those for which the accuracy of the continuum model is sufficient,  $\mathcal{L}_c$ . Upon defining the QCF force operator  $F^{\text{qc}} : \mathcal{Y}_h \rightarrow \mathbb{R}^{\mathbb{Z}}$  by

$$F^{\text{qc}}(y_h) = (F_m^{\text{qc}}(y_h))_{m \in \mathbb{Z}} \quad \text{where} \quad F_m^{\text{qc}}(y_h) = \begin{cases} F_m^a(y_h), & \text{if } \xi_m \in \mathcal{L}_a, \\ F_m^c(y_h), & \text{if } \xi_m \in \mathcal{L}_c, \end{cases}$$

extended periodically, the QCF method is defined by the following nonlinear variational problem:

$$\text{Find } y_h^{\text{qc}} \in \mathcal{Y}_h \text{ s.t.} \quad (F^{\text{qc}}(y_h^{\text{qc}}) + g, v_h)_h = 0 \quad \forall v_h \in \mathcal{U}_h. \quad (11)$$

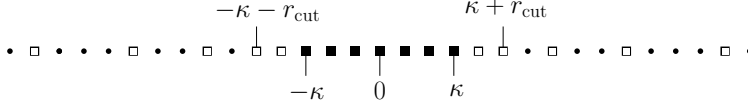
Following previous analyses of the QC method [5, 8, 9, 6] we assume throughout that the atomistic and continuum regions take the form

$$\mathcal{L}_a = \{-\kappa, \dots, \kappa\}, \quad \text{and} \quad \mathcal{L}_c = \mathcal{L}_{\text{rep}} \setminus \mathcal{L}_a, \quad (12)$$

where  $\kappa \geq 1$ . Moreover, we will normally assume that

$$\{-\kappa - r_{\text{cut}}, \dots, \kappa + r_{\text{cut}}\} \subset \mathcal{L}_{\text{rep}}; \quad (13)$$

see Figure 1 for a visualisation of  $\mathcal{L}_a$ ,  $\mathcal{L}_c$ , and condition (13). Condition (13) simplifies both the analysis and the implementation of the QCF method, and, more importantly, it guarantees a superconvergence effect that may otherwise be absent (see Remark 7). Namely, we note that (13) implies that  $F_m^a(y_h) = f_{\xi_m}^a(y_h)$  for all  $\xi_m \in \mathcal{L}_a$ .



**Fig. 1** Visualisation of  $\mathcal{L}_a$  (black squares),  $\mathcal{L}_c$  (white squares), and condition (13), with  $\kappa = 3$  and  $r_{\text{cut}} = 2$ .

For future reference we state explicit formulas for  $f_\xi^a$  and  $F_m^c$ . For all  $y \in \mathcal{Y}$ , and  $r = 1, \dots, r_{\text{cut}}$ , we have  $|D_{-r}y_\xi| = -D_{-r}y_\xi$ , which implies that

$$f_\xi^a(y) = \frac{1}{\varepsilon} \sum_{r=1}^{r_{\text{cut}}} (\phi'(|D_r y_\xi|) - \phi'(|D_{-r} y_\xi|)), \quad \text{and} \quad (14)$$

$$F_m^c(y) = \frac{1}{H_m} (DW(Y'_{m+1}) - DW(Y'_m)). \quad (15)$$

*Remark 3 (The pointwise formulation)* The need for the variational formulation (11) of the QCF method is an artifact of the periodic boundary conditions. Preferably, we would like to state (11) in the “pointwise” form

$$F_m^{\text{qc}}(y_h^{\text{qc}}) + g(X_m) = 0 \quad \text{for } m = 1, \dots, M.$$

However, it was shown in [8] that in some cases  $(F^{\text{qc}}(y_h), 1)_h \neq 0$ , that is  $F^{\text{qc}}$  does not map  $\mathcal{U}_h$  to  $\mathcal{U}_h$ , and hence this “pointwise” formulation may lack a solution. In [8], to overcome this difficulty, a projection operator was used, which results in a formulation that is equivalent to our “strong variational formulation” (11). For problems with Dirichlet boundary conditions this effect does not occur [9].  $\square$

## 2.6 Additional Notation

We conclude this section by reviewing some of the notation used in the previous subsection, and introducing additional notation that will be useful in the remainder of the paper.

### 2.6.1 Interpolant

We note that the standard nodal interpolant does not map  $\mathcal{U}$  to  $\mathcal{U}_h$  and hence we define a modified nodal interpolation operator  $I_h : \mathcal{U} \rightarrow \mathcal{U}_h$  as follows:

$$I_h u \in \mathcal{U}_h \quad \text{s.t.} \quad (I_h u)_{\xi_m} = u_{\xi_m} + C \quad \text{for } m \in \mathbb{Z},$$

where the constant  $C$  is determined through the condition  $(I_h u, 1)_h = 0$ . With a slight abuse of notation, we also define the nodal interpolation operator on  $\mathcal{Y}$ , as

$$I_h(Ax + u) = Ax + I_h u. \quad (16)$$

Upon noting that  $I_h u'$  coincides with the gradient of the standard nodal interpolant of  $u$ , and recalling [26, Thm. A.4, Eq. (74)], we obtain the following interpolation error estimate:

$$\|I_h y' - y'\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m\})} \leq \frac{1}{2} h_m \|y''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m-1\})}. \quad (17)$$

### 2.6.2 Duality

The spaces of linear functionals acting on  $\mathcal{U}$  and  $\mathcal{U}_h$  are denoted, respectively, by  $\mathcal{U}^*$  and  $\mathcal{U}_h^*$ , and both corresponding duality pairings by  $\langle \cdot, \cdot \rangle$ , that is,

$$\langle T, v \rangle \quad \text{for } T \in \mathcal{U}^*, v \in \mathcal{U}, \quad \text{and} \quad \langle T, v_h \rangle \quad \text{for } T \in \mathcal{U}_h^*, v_h \in \mathcal{U}_h.$$

For example, we understand the first variation of the atomistic functional,  $D\Phi_{\text{tot}}^a$ , as an element of  $\mathcal{U}^*$ . However, it can also be applied to coarse test functions from  $\mathcal{U}_h$  and it can then also be understood as an element of  $\mathcal{U}_h^*$ . The same is true for the first variation of the continuum model  $D\Phi_{\text{tot}}^c$ . A force vector  $f^a(y)$  (or the external force vector  $g$ ) can also be understood as an element of  $\mathcal{U}^*$  or  $\mathcal{U}_h^*$  via the interpretation

$$\langle f^a(y), v \rangle = (f^a(y), v)_\varepsilon \quad \text{or} \quad \langle f^a(y), v_h \rangle = (f^a(y), v_h)_\varepsilon.$$

We stress, however, that we always understand  $F^{\text{qc}}(y_h)$  as an element of  $\mathcal{U}_h^*$ .

The topological duals of  $\mathcal{U}^{1,p}$  and  $\mathcal{U}_h^{1,p}$  are, respectively, denoted by  $\mathcal{U}^{-1,p'}$  and  $\mathcal{U}_h^{-1,p'}$ , where  $1/p + 1/p' = 1$ ,  $1 \leq p \leq \infty$ . They are equipped with the usual dual norms (or, negative norms)

$$\|T\|_{\mathcal{U}^{-1,p'}} = \sup_{\substack{v \in \mathcal{U} \\ \|v\|_{\mathcal{U}^{1,p}}=1}} \langle T, v \rangle \quad \text{and} \quad \|T\|_{\mathcal{U}_h^{-1,p'}} = \sup_{\substack{v \in \mathcal{U}_h \\ \|v\|_{\mathcal{U}_h^{1,p}}=1}} \langle T, v \rangle.$$

### 2.6.3 Local bounds on the deformation gradient and on the potential

It will be convenient on several occasions to roughly estimate deformation gradients below, in order to then get rough bounds on (derivatives of) the interaction potential from above. To this end, we define the following notation:

$$\mu_\xi^a(y) = \min_{\substack{\zeta \in \mathbb{Z} \\ |\zeta - \xi| \leq r_{\text{cut}} - 1}} y'_\zeta \quad \text{for } y \in \mathbb{R}^\mathbb{Z}, \quad (18)$$

$$\mu_\xi^{\text{qc}}(y) = \begin{cases} \mu_\xi^a(y), & \text{if } -\kappa \leq \xi \leq \kappa + 1, \\ y'_\xi, & \text{otherwise.} \end{cases} \quad (19)$$

The value  $\mu_\xi^a(y)$  gives a lower bound on  $y'_\zeta$  in the interaction range of the bond  $(\xi - 1, \xi)$ , and  $\mu_\xi^{\text{qc}}(y)$  gives a similar bound, but takes into account that the interaction range is limited to the bond itself in the continuum model.

Given a lower bound  $\mu$  on the local deformation gradient, we can obtain upper bounds on derivatives of the interaction potential as follows:

$$\overline{\phi^{(j)}}(\mu) := \sup_{t \geq \mu} |\phi^{(j)}(t)| \quad \text{for } \mu > 0 \text{ and for } j = 2, 3. \quad (20)$$

### 3 The Atomistic Stress Function

In the language of finite element analysis, (8), (10), (11) might be considered the *strong formulations* of the atomistic, QCL and QCF models, whereas, in the present section, we are deriving corresponding *weak formulations* in terms of stress functions. Model error estimates for the stress functions will then quickly lead to sharp consistency error estimates in negative norms, which occur naturally in the error analysis.

We remark that negative norm techniques for finite difference methods go back to the work of Tikhonov and Samarskii [33], where they were developed for the construction and analysis of finite difference discretizations of diffusion equations with non-smooth coefficients and on non-uniform meshes.

#### 3.1 Derivation of the stress functions

Recall from Section 2.4 the notation  $V_m = v_h(X_m) = v_{h,\xi_m}$  and  $V'_m = (V_m - V_{m-1})/h_m$  for finite element functions  $v_h \in \mathcal{S}_h^1$ . We begin by deriving the weak formulation of the QCL method. A straightforward and standard calculation, starting from (5), gives the following representation of the first variation of  $\Phi^c$ . The formula (23) below is obtained from (21) using summation by parts.

**Proposition 1** *Let  $y_h \in \mathcal{Y}_h$ ; then,*

$$\langle D\Phi^c(y_h), v_h \rangle = \sum_{m=1}^M h_m \Sigma_m^c(y_h) V'_m \quad \text{for all } v_h \in \mathcal{U}_h, \quad (21)$$

where the Cauchy–Born stress function is given by

$$\Sigma_m^c(y_h) = DW(Y'_m),$$

The function  $DW$ , expressed in terms of  $\phi$ , reads

$$DW(F) = \sum_{r=1}^{r_{\text{cut}}} r \phi'(Fr) \quad \text{for } F > 0. \quad (22)$$

Moreover, the forces and stresses of the continuum model (or, QCL model) are related by the formula

$$F_m^c(y_h) = H_m^{-1} [\Sigma_{m+1}^c(y_h) - \Sigma_m^c(y_h)]. \quad (23)$$

In our next result we obtain an analogous representation of the first variation of the atomistic functional  $\Phi^a$ . The main difference is that the stress function for the atomistic model is non-local, that is, it depends on the strains from neighbouring bonds.

**Proposition 2 (The Atomistic Stress Function)** *Let  $y \in \mathcal{Y}$ ; then,*

$$\langle D\Phi^a(y), v \rangle = \varepsilon \sum_{\xi \in \mathcal{L}} \sigma_\xi^a(y) v'_\xi \quad \text{for all } v \in \mathcal{U}, \quad (24)$$

where the atomistic stress function  $\sigma_\xi^a(y)$  is given by

$$\sigma_\xi^a(y) = \sum_{r=1}^{r_{\text{cut}}} \sum_{\zeta=\xi-r}^{\xi-1} \phi'(D_r y_\zeta). \quad (25)$$

Moreover, the atomistic forces and stresses are related by the formula

$$f_\xi^a(y) = \varepsilon^{-1} [\sigma_{\xi+1}^a(y) - \sigma_\xi^a(y)]. \quad (26)$$

*Proof* As a first step we rewrite  $\Phi^a(y)$  as

$$\Phi^a(y) = \varepsilon \sum_{r=1}^{r_{\text{cut}}} \sum_{\zeta=-N+1}^N \phi(D_r y_\zeta),$$

from which we obtain the following representation of  $D\Phi^a(y)$ :

$$\langle D\Phi^a(y), v \rangle = \varepsilon \sum_{r=1}^{r_{\text{cut}}} \sum_{\zeta=-N+1}^N \phi'(D_r y_\zeta) D_r v_\zeta. \quad (27)$$

We now write the long-range finite differences  $D_r v_\zeta = \varepsilon^{-1}(v_{\zeta+r} - v_\zeta)$  in terms of the nearest-neighbour differences  $v'_\xi$ ,

$$D_r v_\zeta = \frac{v_{\zeta+r} - v_\zeta}{\varepsilon} = \sum_{\xi=\zeta+1}^{\zeta+r} v'_\xi.$$

Inserting this formula into (27) we can obtain (24) and (25) by interchanging the order of summation as follows.

If we fix some  $r > 0$ , then we observe that the strain  $v'_\xi$  occurs together with the term  $\phi'(D_r y_\zeta)$  if and only if

$$\zeta + 1 \leq \xi \leq \zeta + r,$$

or equivalently, the term  $\phi'(D_r y_\zeta)$  occurs together with the strain  $v'_\xi$  if and only if

$$\xi - r \leq \zeta \leq \xi - 1.$$

This immediately implies (24) and (25).

To prove (26) we use summation by parts in (24) to arrive at

$$\langle D\Phi^a(y), v \rangle = \sum_{\xi \in \mathcal{L}} v_\xi (\sigma_\xi^a - \sigma_{\xi+1}^a) = \varepsilon \sum_{\xi \in \mathcal{L}} v_\xi \frac{\sigma_\xi^a - \sigma_{\xi+1}^a}{\varepsilon} \quad \text{for all } v \in \mathcal{U}.$$

Since all periodic test functions with mean zero are admitted, this shows that (26) is correct up to some constant  $C$ , that is,

$$f_\xi^a = \frac{\sigma_{\xi+1}^a - \sigma_\xi^a}{\varepsilon} + C. \quad (28)$$

It follows from the translational invariance of  $\Phi^a$  (see, e.g., [8, Eq. (2)]) that

$$\sum_{\xi \in \mathcal{L}} \frac{\partial \Phi^a(y)}{\partial y_\xi} = 0, \quad \text{that is,} \quad \sum_{\xi \in \mathcal{L}} f_\xi^a = 0.$$

Summing (28), and using the periodicity of  $\sigma_\xi^a$ , we obtain that  $C = 0$ .  $\square$

### 3.2 Model error of the Cauchy–Born stress function.

In this section we derive estimates for the difference between the atomistic and continuum stress functions. This result will be a crucial ingredient in the consistency analysis in Section 4.3. We note that at this stage finite element coarsening does not play a role.

**Theorem 1 (Model Error Estimate)** *Recall the definitions of  $DW$  and  $\sigma_\xi^a$  from, respectively, Propositions 1 and 2. Let  $y \in \mathbb{R}^{\mathbb{Z}}$  and let  $\xi \in \mathbb{Z}$  be such that  $\mu_\xi^a(y) > 0$ , where  $\mu_\xi^a$  is defined in (18); then,*

$$|\sigma_\xi^a(y) - DW(y'_\xi)| \leq \varepsilon^2 \sum_{s=\pm 1}^{\pm(r_{\text{cut}}-1)} \left\{ K_{\xi,s}^{(2)} \left| \frac{y'_{\xi+s} - 2y'_\xi + y'_{\xi-s}}{(s\varepsilon)^2} \right| + K_{\xi,s}^{(3)} \left| \frac{y'_{\xi+s} - y'_\xi}{s\varepsilon} \right|^2 \right\}, \quad (29)$$

where the decay factors  $K_{\xi,s}^{(j)}$ ,  $j = 2, 3$ , are defined by

$$K_{\xi,s}^{(j)} = \frac{s^2}{2} \sum_{r=|s|+1}^{r_{\text{cut}}} (r - |s|) \overline{\phi^{(j)}}(r\mu_\xi^a(y)), \quad (30)$$

and  $\overline{\phi^{(j)}}$  is defined in (20).

*Remark 4* The decay factors  $K_{\xi,s}^{(j)}$  describe the rate of decay of the interaction potential. They quantify the observation that, even though the model error estimate does depend nonlocally on second and third finite difference quotients, the impact of longer-range dependence decays rapidly provided the interaction potential decays rapidly as well.

We also note that an inspection of the proof of Theorem 1 shows that the term  $r\mu_\xi^a(y)$  may be replaced by  $ry'_\xi$  in the definition of the constant  $K_{\xi,s}^{(2)}$ , but not in the definition of  $K_{\xi,s}^{(3)}$ . Moreover we will use  $K_{\xi,s}^{(2)}$  below in situations where  $ry'_\xi$  is not sufficient.  $\square$

*Proof* We set  $\mu_\xi^a := \mu_\xi^a(y)$  and  $\sigma_\xi^a := \sigma_\xi^a(y)$  throughout. Recalling the formulas (22) and (25), we obtain

$$\begin{aligned} \sigma_\xi^a - DW(y'_\xi) &= \sum_{r=1}^{r_{\text{cut}}} \sum_{\zeta=\xi-r}^{\xi-1} \phi'(D_r y_\zeta) - \sum_{r=1}^{r_{\text{cut}}} r \phi'(r y'_\xi) \\ &= \sum_{r=1}^{r_{\text{cut}}} \sum_{\zeta=\xi-r}^{\xi-1} \{\phi'(D_r y_\zeta) - \phi'(r y'_\xi)\}. \end{aligned} \quad (31)$$

We note that the stated model error estimate is second order in  $\varepsilon$ , and hence we need to expand the difference  $\phi'(D_r y_\zeta) - \phi'(r y'_\xi)$  to second order. There exists  $\theta_{r,\zeta} \in \text{conv}\{D_r y_\zeta, r y'_\xi\}$ , in particular  $\theta_{r,\zeta} \geq r \mu_\xi^a$ , such that

$$\phi'(D_r y_\zeta) - \phi'(r y'_\xi) = \phi''(r y'_\xi)(D_r y_\zeta - r y'_\xi) + \frac{1}{2} \phi'''(\theta_{r,\zeta})(D_r y_\zeta - r y'_\xi)^2.$$

Inserting this expansion into (31) yields

$$\begin{aligned} |\sigma_\xi^a - DW(y'_\xi)| &\leq \left\{ \sum_{r=1}^{r_{\text{cut}}} |\phi''(r y'_\xi)| \left| \sum_{\zeta=\xi-r}^{\xi-1} (D_r y_\zeta - r y'_\xi) \right| \right\} \\ &\quad + \left\{ \frac{1}{2} \sum_{r=1}^{r_{\text{cut}}} \sum_{\zeta=\xi-r}^{\xi-1} |\phi'''(\theta_{r,\zeta})| (D_r y_\zeta - r y'_\xi)^2 \right\} =: T_1 + T_2. \end{aligned}$$

*Estimating  $T_2$ .* We split the long-range interaction  $D_r y_\zeta$  into short range interactions  $y'_\eta$ , and then employ the Cauchy–Schwarz inequality to bound

$$(D_r y_\zeta - r y'_\xi)^2 = \left( \sum_{\eta=\zeta+1}^{\zeta+r} (y'_\eta - y'_\xi) \right)^2 \leq r \sum_{\eta=\zeta+1}^{\zeta+r} |y'_\eta - y'_\xi|^2,$$

to obtain

$$T_2 \leq \frac{1}{2} \sum_{r=1}^{r_{\text{cut}}} \sum_{\zeta=\xi-r}^{\xi-1} r |\phi'''(\theta_{r,\zeta})| \sum_{\eta=\zeta+1}^{\zeta+r} |y'_\eta - y'_\xi|^2.$$

Next, we change the order of summation from  $(r, \zeta, \eta)$  to  $(\eta, r, \zeta)$ . To this end, we consider the following equivalences,

$$\begin{aligned} \left\{ \begin{array}{l} 1 \leq r \leq r_{\text{cut}} \\ \xi - r \leq \zeta \leq \xi - 1 \\ \zeta + 1 \leq \eta \leq \zeta + r \end{array} \right\} &\Leftrightarrow \left\{ \begin{array}{l} 1 \leq r \leq r_{\text{cut}} \\ \xi - (r - 1) \leq \eta \leq \xi + (r - 1) \\ (\eta - r) \vee (\xi - r) \leq \zeta \leq (\eta - 1) \wedge (\xi - 1) \end{array} \right\} \\ &\Leftrightarrow \left\{ \begin{array}{l} \xi - (r_{\text{cut}} - 1) \leq \eta \leq \xi + (r_{\text{cut}} - 1) \\ |\xi - \eta| + 1 \leq r \leq r_{\text{cut}} \\ (\eta \vee \xi) - r \leq \zeta \leq (\eta \wedge \xi) - 1 \end{array} \right\}, \end{aligned} \quad (32)$$

where we have used the notation  $a \wedge b = \min(a, b)$  and  $a \vee b = \max(a, b)$ . Employing (32) we obtain

$$T_2 \leq \frac{1}{2} \sum_{\eta=\xi-(r_{\text{cut}}-1)}^{\xi+(r_{\text{cut}}-1)} |y'_\eta - y'_\xi|^2 \left\{ \sum_{r=|\xi-\eta|+1}^{r_{\text{cut}}} \sum_{\zeta=(\eta \vee \xi)-r}^{(\eta \wedge \xi)-1} |\phi'''(\theta_{r,\zeta})| \right\}. \quad (33)$$

Using the fact that  $\theta_{r,\zeta} \geq r\mu_\xi^a$ , we deduce the estimate

$$|\phi'''(\theta_{r,\zeta})| \leq \sup_{t \geq r\mu_\xi^a} |\phi'''(t)| = \overline{\phi'''}(r\mu_\xi^a),$$

and hence,

$$\begin{aligned} \sum_{\zeta=(\eta \vee \xi)-r}^{(\eta \wedge \xi)-1} |\phi'''(\theta_{r,\zeta})| &\leq \overline{\phi'''}(r\mu_\xi^a) \cdot [((\eta \wedge \xi) - 1) - ((\eta \vee \xi) - r) + 1] \\ &= \overline{\phi'''}(r\mu_\xi^a) \cdot [r - |\eta - \xi|]. \end{aligned}$$

Setting  $s = \eta - \xi$  in (33), and noting that all inner terms disappear for  $s = 0$ , we obtain

$$|\sigma_\xi^a - DW(y'_\xi)| \leq \sum_{s=\pm 1}^{\pm(r_{\text{cut}}-1)} \left\{ \frac{1}{2} \sum_{r=|s|+1}^{r_{\text{cut}}} (r - |s|) \overline{\phi'''}(r\mu_\xi^a) \right\} |y'_{\xi+s} - y'_\xi|^2.$$

Rescaling the term  $|y'_{\xi+s} - y'_\xi|^2$  by the factor  $(\varepsilon s)^2$  gives the second group in (29).

*Estimating  $T_1$ .* We will use symmetries to carefully estimate the term

$$T_{1,r} := \sum_{\zeta=\xi-r}^{\xi-1} (D_r y_\zeta - r y'_\zeta),$$

to arrive at a third finite difference. For illustration we briefly consider the special case  $r = 2$ . In that case, we have

$$\begin{aligned} T_{1,2} &= \frac{y_\xi - y_{\xi-2}}{\varepsilon} - 4y'_\xi + \frac{y_{\xi+1} - y_{\xi-1}}{\varepsilon} \\ &= (y'_{\xi-1} + y'_\xi) - 4y'_\xi + (y'_\xi + y'_{\xi+1}) \\ &= y'_{\xi+1} - 2y'_\xi + y'_{\xi-1}, \end{aligned}$$

which is indeed a third finite difference. For general  $r$ , a similar but more involved calculation, which is carried out in detail below, yields

$$T_{1,r} = \sum_{s=1}^{r-1} (r-s)(y'_{\xi+s} - 2y'_\xi + y'_{\xi-s}). \quad (34)$$

Inserting (34) into the definition of  $T_1$ , and rescaling the third finite difference by  $(s\varepsilon)^2$ , we obtain

$$T_1 \leq \varepsilon^2 \sum_{r=2}^{r_{\text{cut}}} |\phi''(r y'_\xi)| \sum_{s=1}^{r-1} s^2 (r-s) \left| \frac{y'_{\xi+s} - 2y'_\xi + y'_{\xi-s}}{(s\varepsilon)^2} \right|.$$



Exchanging the order of summation, we arrive at the estimate

$$T_1 \leq \varepsilon^2 \sum_{s=1}^{r_{\text{cut}}-1} \left\{ s^2 \sum_{r=s+1}^{r_{\text{cut}}} (r-s) |\phi''(ry'_\xi)| \right\} \left| \frac{y'_{\xi+s} - 2y'_\xi + y'_{\xi-s}}{(s\varepsilon)^2} \right|.$$

Estimating  $|\phi''(ry'_\xi)|$  above by  $\overline{\phi''}(r\mu_\xi^a)$  and replacing the first sum from  $s=1$  to  $(r_{\text{cut}}-1)$  with a sum from  $-(r_{\text{cut}}-1)$  to  $(r_{\text{cut}}-1)$ , thus gaining a factor of  $1/2$ , we obtain the first group in (29).

(Proof of (34)) We rewrite the long-range difference as a sum of discrete strains, to obtain

$$T_{1,r} = \sum_{\zeta=\xi-r}^{\xi-1} \left( \frac{y_{\zeta+r} - y_\zeta}{\varepsilon} - ry'_\xi \right) = \sum_{\zeta=\xi-r}^{\xi-1} \sum_{\eta=\zeta+1}^{\zeta+r} (y'_\eta - y'_\xi).$$

Next, we interchange the order of summation,

$$T_{1,r} = \sum_{\eta=\xi-(r-1)}^{\xi+(r-1)} (y'_\eta - y'_\xi) \sum_{\zeta=(\eta-r) \vee (\xi-r)}^{(\eta-1) \wedge (\xi-1)} 1 = \sum_{\eta=\xi-(r-1)}^{\xi+(r-1)} (y'_\eta - y'_\xi) (r - |\eta - \xi|).$$

Combining the terms for  $\eta = \xi - s$  and  $\eta = \xi + s$ ,  $s = 1, \dots, r-1$ , yields

$$T_{1,r} = \sum_{s=1}^{r-1} (y'_{\xi+s} - 2y'_\xi + y'_{\xi-s})(r-s),$$

which is precisely the desired formula.  $\square$

## 4 Analysis of the QCF Method

### 4.1 Weak form of the QCF method

For our analysis of the QCF method, we first need to derive its “weak” formulation, by performing summation by parts on the strong form of the QCF equation (11). However, before we can state the result in a convenient way we need to introduce some additional notation.

We use  $\underline{K}, \overline{K} \in \{1, \dots, M\}$  to denote the indices of the degrees of freedom corresponding to the interface atoms  $-\kappa, \kappa$ , that is,

$$\xi_{\underline{K}} = -\kappa, \quad \text{and} \quad \xi_{\overline{K}} = \kappa.$$

The set of indices of finite elements  $(X_{m-1}, X_m)$  that belong, respectively, to the atomistic and continuum regions are defined as

$$\begin{aligned} \mathcal{M}_a &= \{\underline{K}, \dots, \overline{K} + 1\} & \text{and} & \quad \mathcal{M}_c = \{1, \dots, M\} \setminus \mathcal{M}_a. \\ &= \{m : \xi_{m-1} \in \mathcal{L}_a \text{ or } \xi_m \in \mathcal{L}_a\}, \end{aligned} \quad (35)$$

Note that we think of the interface elements  $(X_{K-1}, X_{\underline{K}})$  and  $(X_{\overline{K}}, X_{\overline{K}+1})$  as belonging to the atomistic region. Finally, in order to unify the notation, we will also define

$$\Sigma_m^a(y_h) := \sigma_{\xi_m}^a(y_h) \quad \text{for } y_h \in \mathcal{Y}_h \text{ and for } m \in \mathcal{M}_a. \quad (36)$$

With this notation, we obtain the following result, which is a nonlinear version of [9, Lemma 1]. Our preparations in Section 3 make it straightforward to generalize the formulation and proof of this result.

**Proposition 3** *Let  $y_h \in \mathcal{Y}_h$  and define  $\Sigma_m^{a/c} = \Sigma_m^{a/c}(y_h)$ . Then, for all  $v_h \in \mathcal{U}_h$ ,*

$$\begin{aligned} -(F^{\text{qc}}(y_h), v_h)_h &= \sum_{m \in \mathcal{M}_a} \varepsilon V'_m \Sigma_m^a + \sum_{m \in \mathcal{M}_c} h_m V'_m \Sigma_m^c \\ &\quad - V_{\underline{K}-1}(\Sigma_{\underline{K}}^c - \Sigma_{\underline{K}}^a) + V_{\overline{K}+1}(\Sigma_{\overline{K}+1}^c - \Sigma_{\overline{K}+1}^a). \end{aligned} \quad (37)$$

*Proof* We begin by inserting (23) and (26) into (11), using nodal notation also in the atomistic region (note that, in view of Remark 2 and (13), we have  $F_m(y_h) = f_{\xi_m}(y_h)$  for  $\xi_m \in \mathcal{L}_a$ ), to obtain

$$-(F^{\text{qc}}(y_h), v_h)_h = \sum_{\xi_m \in \mathcal{L}_a} V_m(\Sigma_m^a - \Sigma_{m+1}^a) + \sum_{\xi_m \in \mathcal{L}_c} V_m(\Sigma_m^c - \Sigma_{m+1}^c).$$

We now consider the two “connected components” of  $\mathcal{L}_a$  and  $\mathcal{L}_c$  and perform summation by parts in each such component separately.

Let  $\underline{m} = \underline{K} + 1$  and  $\overline{m} = \overline{K} - 1 + M$ , then, using periodicity,

$$\begin{aligned} \sum_{\xi_m \in \mathcal{L}_c} V_m(\Sigma_m^c - \Sigma_{m+1}^c) &= \sum_{m=\underline{m}}^{\overline{m}} V_m(\Sigma_m^c - \Sigma_{m+1}^c) \\ &= \sum_{m=\underline{m}}^{\overline{m}} V_m \Sigma_m^c - \sum_{m=\underline{m}+1}^{\overline{m}+1} V_{m-1} \Sigma_m^c \\ &= \sum_{m=\underline{m}+1}^{\overline{m}} h_m V'_m \Sigma_m^c - V_{\overline{m}} \Sigma_{\overline{m}+1}^c + V_{\underline{m}} \Sigma_{\underline{m}}^c. \end{aligned}$$

Inserting the definitions of  $\underline{m}$ ,  $\overline{m}$ , and  $\mathcal{M}_c$ , we obtain

$$\sum_{\xi_m \in \mathcal{L}_c} V_m(\Sigma_m^c - \Sigma_{m+1}^c) = \sum_{m \in \mathcal{M}_c} h_m V'_m \Sigma_m^c - V_{\underline{K}-1} \Sigma_{\underline{K}}^c + V_{\overline{K}+1} \Sigma_{\overline{K}+1}^c.$$

An analogous calculation in the atomistic region, where  $h_m = \varepsilon$ , gives

$$\sum_{\xi_m \in \mathcal{L}_a} V_m(\Sigma_m^a - \Sigma_{m+1}^a) = \sum_{m \in \mathcal{M}_a} \varepsilon V'_m \Sigma_m^a - V_{\overline{K}+1} \Sigma_{\overline{K}+1}^a + V_{\underline{K}-1} \Sigma_{\underline{K}}^a.$$

Combining the two foregoing formulas gives the desired result.  $\square$

*Remark 5* Our formulation of Proposition 3 in terms of the continuum and atomistic stress functions reveals that the interface terms in the weak form of the QCF method, first observed in [9], are simply jumps of the stress. In multiphysics continuum mechanics one usually requires that the (normal component of) the jump of the stress vanishes, which would correspond to removing the interface terms from the variational formulation. The analysis in [9] has shown that these terms are the origin of the poor stability properties of the QCF method. Hence, in Section 5 we will investigate a new coupling method where these terms are indeed removed.  $\square$

## 4.2 Stability

The question of stability of the QCF method is exceedingly subtle and a complete investigation would exceed the scope of this paper. The difficulties we are facing are exclusively related to the interface terms appearing in the weak form (37). In the present paper, we will be satisfied to assume that nearest-neighbour interactions strongly dominate all other interactions. Sharper stability analyses are the focus of ongoing research. In [10], for example, several sharp stability estimates are established in a special situation (linearization around the homogeneous deformation  $y = Ax$ ); however, the methods developed in that reference do not obviously extend to large deformations.

Note that we make no claim in the following theorem, whether  $\gamma_f(y_h)$  is positive or not. We discuss in Remark 6 whether it is reasonable to expect this, and in our a priori error analysis in Section 4.4 we will formulate this as an assumption.

**Theorem 2** *Let  $y_h \in \mathcal{Y}_h$ ; then,*

$$\inf_{\substack{u_h \in \mathcal{U}_h \\ \|u_h\|_{\mathcal{U}^{1,\infty}}=1}} \sup_{\substack{v_h \in \mathcal{U}_h \\ \|v_h\|_{\mathcal{U}^{1,1}}=1}} \left( -DF^{\text{qc}}(y_h)u_h, v_h \right)_h \geq \gamma_f(y_h), \quad \text{where} \quad (38)$$

$$\gamma_f(y_h) = \min_{\xi \in \mathcal{L}} \frac{1}{2} \left\{ \phi''(y'_{h,\xi}) - \sum_{r=2}^{r_{\text{cut}}} r^2 \overline{\phi''}(r\mu_{\xi}^{\text{qc}}(y_h)) \right\}$$

$$- \max_{\xi \in \{-\kappa, \kappa+1\}} \frac{1}{2} \left\{ \sum_{r=2}^{r_{\text{cut}}} r(r-1) \overline{\phi''}(r\mu_{\xi}^{\text{a}}(y_h)) \right\} - \varepsilon C_1(y_h), \quad \text{and}$$

$$C_1(y_h) = \max_{\xi \in \{-\kappa, \kappa+1\}} \sum_{s=\pm 1}^{\pm(r_{\text{cut}}-1)} |s|^{-1} K_{\xi,s}^{(3)} \left| \frac{y'_{h,\xi+s} - y'_{h,\xi}}{s\varepsilon} \right|.$$

The decay factors  $K_{\xi,s}^{(3)}$  are defined in (30), and the functions  $\overline{\phi^{(j)}}$  in (20).

Many of the techniques we use in the proof of this result are closely related to those used in [4, 9, 8, 26]. We begin by computing a “weak form” of the linearization of  $F^{\text{qc}}$ . To this end, recall the definitions of  $\mathcal{M}_a, \mathcal{M}_c$  from the previous section.

**Proposition 4** Let  $y_h \in \mathcal{Y}_h$ , and  $u_h, v_h \in \mathcal{U}_h$ ; then,

$$\begin{aligned} -(DF^{\text{qc}}(y_h)u_h, v_h)_h &= \sum_{m \in \mathcal{M}_a} \sum_{n=1}^M h_m \mathcal{H}_{m,n}^a V'_m U'_n + \sum_{m \in \mathcal{M}_c} \sum_{n=1}^M h_m \mathcal{H}_{m,n}^c V'_m U'_n \\ &\quad - V_{\underline{K}-1} \sum_{n=1}^M (\mathcal{H}_{\underline{K},n}^c - \mathcal{H}_{\underline{K},n}^a) U'_n + V_{\overline{K}+1} \sum_{n=1}^M (\mathcal{H}_{\overline{K}+1,n}^c - \mathcal{H}_{\overline{K}+1,n}^a) U'_n, \end{aligned} \quad (39)$$

where

$$\begin{aligned} \mathcal{H}_{m,n}^c &= \begin{cases} D^2 W(Y'_m), & \text{if } m = n, \\ 0, & \text{if } m \neq n, \end{cases} \quad \text{and} \\ \mathcal{H}_{m,n}^a &= \sum_{r=|\xi_m - \xi_n|_{\#} + 1}^{r_{\text{cut}}} \sum_{\zeta=(\xi_m \vee \xi_n) - r}^{(\xi_m \wedge \xi_n) - 1} \phi''(D_r y_{\zeta}), \end{aligned}$$

with the notation  $|\xi_m - \xi_n|_{\#} := \min\{|\xi_m - \xi_n|, |\xi_m - \xi_{n+M}|, |\xi_m - \xi_{n-M}|\}$ .

*Proof* It is easy to see that

$$D\Sigma_m^c(y_h)u_h = D^2 W(Y'_m)U'_m,$$

which immediately leads to the definition of  $\mathcal{H}^c$ .

The corresponding formula for  $D\Sigma_m^a$  is more complicated. For ease of notation, we replace  $\xi_m$  by  $\xi$ ,  $\xi_n$  by  $\eta$ , and  $y_h, u_h, v_h$  by  $y, u, v$ . Linearization of  $\sigma_{\xi}^a(y)$  yields

$$\langle D\sigma_{\xi}^a(y), u \rangle = \sum_{r=1}^{r_{\text{cut}}} \sum_{\zeta=\xi-r}^{\xi-1} \phi''(D_r y_{\zeta}) D_r u_{\zeta} = \sum_{r=1}^{r_{\text{cut}}} \sum_{\zeta=\xi-r}^{\xi-1} \phi''(D_r y_{\zeta}) \sum_{\eta=\zeta+1}^{\zeta+r} u'_{\eta}.$$

Using (32) to rearrange the order of summation, we obtain

$$\langle D\sigma_{\xi}^a(y), u \rangle = \sum_{\eta=\xi-(r_{\text{cut}}-1)}^{\xi+(r_{\text{cut}}-1)} u'_{\eta} \left\{ \sum_{\zeta=(\xi \vee \eta)-r}^{(\xi \wedge \eta)-1} \phi''(D_r y_{\zeta}) \right\},$$

which gives the stated formula for  $\mathcal{H}_{m,n}^a$ .

Inserting the linearizations of  $\Sigma_m^{\text{a/c}}$  into the weak form (37) gives the stated weak form of the linearized QCF operator.  $\square$

Our proof of the stability result will be based on the following basic inf-sup stability lemma.

**Lemma 1** Let  $(\mathcal{J}_{m,n})_{m,n=1}^M \subset \mathbb{R}$  satisfy  $\mathcal{J}_{m,m} > 0$  for  $m = 1, \dots, M$ ; then,

$$\inf_{\substack{u_h \in \mathcal{U}_h \\ \|u_h\|_{\mathcal{U}^1, \infty} = 1}} \sup_{\substack{v_h \in \mathcal{U}_h \\ \|v_h\|_{\mathcal{U}^1, 1} = 1}} \sum_{m,n=1}^M h_m \mathcal{J}_{m,n} U'_n V'_m \geq \min_{m=1, \dots, M} \frac{1}{2} \left( \mathcal{J}_{mm} - \sum_{n \neq m} |\mathcal{J}_{mn}| \right).$$

*Proof* Fix  $u_h \in \mathcal{U}_h$  with  $\|u'_h\|_{\ell^\infty} = 1$ , and let  $p, q \in \{1, \dots, M\}$  such that  $U'_p = \max U'_n$  and  $U'_q = \min U'_n$ . Then  $U'_p > 0$  and  $U'_q < 0$ , and we can define  $v_h \in \mathcal{U}_h$  via the condition

$$V'_n = \begin{cases} (2h_p)^{-1}, & n = p, \\ -(2h_q)^{-1}, & n = q, \\ 0, & \text{otherwise.} \end{cases}$$

Inserting this test function immediately gives the stated lower bound.  $\square$

To be able to apply the previous lemma, we now need to express the interface terms in (39) in terms of gradients as a direct estimate through embedding inequalities would lead to grossly suboptimal bounds. Following [8, Appendix A], we use periodic Heaviside functions to rewrite  $V_{\bar{K}+1}$  and  $V_{\bar{K}-1}$  in terms of gradients. We will use the fact (see [8, Eq. (A.2)]) that, for all  $v \in \mathcal{U}$ ,

$$v_0 = (s, v')_\varepsilon, \quad \text{where} \quad s_\xi = \begin{cases} -\frac{1}{2}(1 - \varepsilon\xi) - \frac{\varepsilon}{4}, & \xi \geq 1, \\ \frac{1}{2}(1 + \varepsilon\xi) + \frac{5\varepsilon}{4}, & \xi < 1. \end{cases} \quad (40)$$

We note that the arbitrary constant factor in  $s$  is chosen so that  $s \in \mathcal{U}$ .

**Proposition 5** *Let  $y_h \in \mathcal{Y}_h$  and  $\mathcal{H}_{m,n}^a, \mathcal{H}_{m,n}^c$  defined as in Proposition 4; then,*

$$\begin{aligned} -(DF^{\text{qc}}(y_h)u_h, v_h) &= \sum_{m \in \mathcal{M}_a} \sum_{n=1}^M h_m (\mathcal{H}_{m,n}^a + \mathcal{H}_{m,n}^i) V'_m U'_n \\ &\quad + \sum_{m \in \mathcal{M}_c} \sum_{n=1}^M h_m (\mathcal{H}_{m,n}^c + \mathcal{H}_{m,n}^i) V'_m U'_n, \end{aligned} \quad (41)$$

where  $(\mathcal{H}_{m,n}^i)_{m,n=1}^M$  is defined as follows:

$$\begin{aligned} \mathcal{H}_{m,n}^i &= \bar{S}_m (\mathcal{H}_{\bar{K}+1,n}^c - \mathcal{H}_{\bar{K}+1,n}^a) - \underline{S}_m (\mathcal{H}_{\bar{K},n}^c - \mathcal{H}_{\bar{K},n}^a) \\ \text{with } \bar{S}_m &= \sum_{\xi=\xi_{m-1}}^{\xi_m} \frac{\varepsilon}{h_m} s_{\xi-\kappa-1}, \quad \text{and } \underline{S}_m = \sum_{\xi=\xi_{m-1}}^{\xi_m} \frac{\varepsilon}{h_m} s_{\xi+\kappa+1}. \end{aligned}$$

*Proof* Using (40) we obtain

$$\begin{aligned} V_{\bar{K}+1} &= v_{\kappa+1} = \sum_{\xi=-N+1}^N \varepsilon s_{\xi-\kappa-1} v'_\xi \\ &= \sum_{m=1}^M h_m V'_m \left\{ \sum_{\xi=\xi_{m-1}+1}^{\xi_m} \frac{\varepsilon}{h_m} s_{\xi-\kappa-1} \right\} \\ &= \sum_{m=1}^M h_m V'_m \bar{S}_m, \end{aligned}$$

and similarly,

$$V_{\underline{K}-1} = \sum_{m=1}^M h_m V'_m \underline{S}_m.$$

The result follows after inserting these formulas into (39).  $\square$

The final step, before we can state the proof of the stability theorem, is to compute explicit bounds on the coefficients  $\mathcal{H}_{m,n}^a$ ,  $\mathcal{H}_{m,n}^c$ , and  $\mathcal{H}_{m,n}^i$ .

**Lemma 2** *Let  $y_h \in \mathcal{Y}_h$ , let  $\mathcal{H}_{m,n}^a$  be defined as in Proposition 4, and  $\mathcal{H}_{m,n}^i$  as in Proposition 5; then,*

$$\mathcal{H}_{m,m}^a - \sum_{n \neq m} |\mathcal{H}_{m,n}^a| \geq \phi''(Y'_m) - \sum_{r=2}^{r_{\text{cut}}} r^2 \bar{\phi}''(r \mu_{\xi_m}^a(y_h)), \quad \text{for all } m \in \mathcal{M}_a. \quad (42)$$

Moreover, recalling the definition of  $K_{\xi,s}^{(3)}$  in (30), we have the bound

$$\begin{aligned} \sum_{n=1}^M |\mathcal{H}_{mn}^i| &\leq \max_{\xi \in \{-\kappa, \kappa+1\}} \left\{ 2 \sum_{r=1}^{r_{\text{cut}}} r(r-1) \bar{\phi}''(r \mu_{\xi}^a(y_h)) \right. \\ &\quad \left. + \varepsilon \sum_{s=\pm 1}^{\pm(r_{\text{cut}}-1)} \frac{2}{|s|} K_{\xi,s}^{(3)} \left| \frac{y'_{h,\xi+s} - y'_{h,\xi}}{s\varepsilon} \right| \right\} \quad (43) \\ &\quad \text{for all } m = 1, \dots, M. \end{aligned}$$

*Proof (Proof of (42))* First, we estimate the off-diagonal entries  $\mathcal{H}_{m,n}^a$  with  $n = m + k$ ,  $k = 1, \dots, r_{\text{cut}} - 1$ :

$$|\mathcal{H}_{m,m+k}^a| \leq \sum_{r=k+1}^{r_{\text{cut}}} \sum_{\zeta=\xi_{m+k}-r}^{\xi_m-1} |\phi''(D_r y_{\zeta})| \leq \sum_{r=k+1}^{r_{\text{cut}}} (r-k) \bar{\phi}''(r \mu_{\xi_m}^a(y_h)).$$

The same estimate holds for  $\mathcal{H}_{m,m-k}^a$ . Thus, summing over all off-diagonal entries gives

$$\begin{aligned} \sum_{n \neq m} |\mathcal{H}_{m,n}^a| &\leq 2 \sum_{k=1}^{r_{\text{cut}}-1} \sum_{r=k+1}^{r_{\text{cut}}} (r-k) \bar{\phi}''(r \mu_{\xi_m}^a(y_h)) \\ &= \sum_{r=2}^{r_{\text{cut}}} \sum_{k=1}^{r-1} 2(r-k) \bar{\phi}''(r \mu_{\xi_m}^a(y_h)) \\ &= \sum_{r=2}^{r_{\text{cut}}} r(r-1) \bar{\phi}''(r \mu_{\xi_m}^a(y_h)). \quad (44) \end{aligned}$$

Similarly, we can estimate the diagonal entry  $\mathcal{H}_{mm}^a$  as follows:

$$\mathcal{H}_{mm}^a = \sum_{r=1}^{r_{\text{cut}}} \sum_{\zeta=\xi_m-r}^{\xi_m-1} \phi''(D_r y_{\zeta}) \geq \phi''(Y'_m) - \sum_{r=2}^{r_{\text{cut}}} r \bar{\phi}''(r \mu_{\xi_m}^a(y_h)).$$

Combining this with the previous estimate, we obtain the stated lower bound.

(Proof of (43)) From the definition of  $\mathcal{H}_{mn}^i$  we have

$$\sum_{n=1}^M |\mathcal{H}_{mn}^i| \leq (|\bar{S}_m| + |\underline{S}_m|) \max_{m \in \{\underline{K}, \bar{K}+1\}} \sum_{n=1}^M |\mathcal{H}_{\bar{K}+1,n}^c - \mathcal{H}_{\underline{K}+1,n}^a|. \quad (45)$$

Next, using the fact that  $|s_{\xi-\kappa-1}| + |s_{\xi+\kappa+1}| \leq 1$  for all  $\xi$  (cf. [8, App. A, Proof of Thm. 4.4]), we estimate

$$|\bar{S}_m| + |\underline{S}_m| \leq \frac{\varepsilon}{h_m} \sum_{\xi=\xi_{m-1}+1}^{\xi_m} (|s_{\xi-\kappa-1}| + |s_{\xi+\kappa+1}|) \leq \frac{\varepsilon}{h_m} \sum_{\xi=\xi_{m-1}+1}^{\xi_m} 1 = 1. \quad (46)$$

Thus, we are left to estimate  $|\mathcal{H}_{mn}^c - \mathcal{H}_{mn}^a|$ . To this end, we first consider

$$\begin{aligned} |\mathcal{H}_{mm}^c - \mathcal{H}_{mm}^a| &= \left| \sum_{r=1}^{r_{\text{cut}}} r^2 \phi''(rY'_m) - \sum_{r=1}^{r_{\text{cut}}} \sum_{r=1}^{r_{\text{cut}}} \sum_{\zeta=\xi_m-r}^{\xi_m-1} \phi''(D_r y_\zeta) \right| \\ &\leq \sum_{r=2}^{r_{\text{cut}}} r(r-1) \bar{\phi}''(rY'_m) + \sum_{r=2}^{r_{\text{cut}}} \sum_{\zeta=\xi_m-r}^{\xi_m-1} |\phi''(rY'_m) - \phi''(D_r y_\zeta)|. \end{aligned}$$

Furthermore, a calculation along the same lines as the estimation of  $T_2$  in the proof of Theorem 1 yields

$$\sum_{r=2}^{r_{\text{cut}}} \sum_{\zeta=\xi_m-r}^{\xi_m-1} |\phi''(rY'_m) - \phi''(D_r y_\zeta)| \leq \varepsilon \sum_{s=\pm 1}^{\pm(r_{\text{cut}}-1)} \frac{2}{|s|} K_{\xi_m,s}^{(3)} \left| \frac{y'_{h,\xi_m+s} - y'_{h,\xi_m}}{s\varepsilon} \right|. \quad (47)$$

Since  $\mathcal{H}_{mn}^c = 0$  for  $m \neq n$ , we have

$$\sum_{n \neq m} |\mathcal{H}_{mn}^c - \mathcal{H}_{mn}^a| = \sum_{n \neq m} |\mathcal{H}_{mn}^a|,$$

and we can use (44) and (47) to deduce that, for  $m \in \{\underline{K}, \bar{K}+1\}$ ,

$$\begin{aligned} \sum_{n=1}^M |\mathcal{H}_{m,n}^a - \mathcal{H}_{m,n}^c| &\leq 2 \sum_{r=2}^{r_{\text{cut}}} r(r-1) \bar{\phi}''(r\mu_{\xi_m}^a(y_h)) \\ &\quad + \varepsilon \sum_{s=\pm 1}^{\pm(r_{\text{cut}}-1)} \frac{2}{|s|} K_{\xi_m,s}^{(3)} \left| \frac{y'_{h,\xi_m+s} - y'_{h,\xi_m}}{s\varepsilon} \right|. \end{aligned} \quad (48)$$

Combining (48), with (45) and (46), we immediately obtain (43).  $\square$

We are now in a position to conclude the proof of Theorem 2.

*Proof (Proof of Theorem 2)* We begin by noting that we have the trivial bound

$$D^2W(Y'_m) = \sum_{r=1}^{r_{\text{cut}}} r^2 \phi''(rY'_m) \geq \phi''(Y'_m) - \sum_{r=2}^{r_{\text{cut}}} r^2 \phi''(r\mu_{\xi_m}^{\text{qc}}(y_h)). \quad (49)$$

If we now define

$$\mathcal{J}_{mn} = \begin{cases} \mathcal{H}_{mn}^{\text{a}} + \mathcal{H}_{mn}^{\text{i}}, & m \in \mathcal{M}_{\text{a}}, \\ \mathcal{H}_{mn}^{\text{c}} + \mathcal{H}_{mn}^{\text{i}}, & m \in \mathcal{M}_{\text{c}}, \end{cases}$$

then (42), (49), and (48) imply that

$$\mathcal{J}_{mm} - \sum_{n \neq m} |\mathcal{J}_{mn}| \geq 2\gamma_{\text{f}}(y_h) \quad \text{for all } m = 1, \dots, M.$$

Applying Lemma 1 gives the result.  $\square$

*Remark 6* To understand how sharp the stability result, Theorem 2, is we consider the case of second-neighbour pair interactions ( $r_{\text{cut}} = 2$ ) with Morse potential  $\phi(t) = e^{-2\alpha(t-1)} - 2e^{-\alpha(t-1)}$ , and homogeneous deformations  $y = Ax$ , where  $A$  is chosen sufficiently large so that  $\phi''(2A) \leq 0$ . In that case it was shown in [6] that the atomistic Hessian  $D^2\Phi^{\text{a}}(Ax)$  and the QCL Hessian  $D^2\Phi^{\text{c}}(Ax)$  are positive definite if and only if

$$\phi''(A) + 4\phi''(2A) > 0.$$

(As a matter of fact, for the atomistic Hessian an  $O(\varepsilon^2)$  term should be added to the left-hand side.) By contrast, if  $\phi''(2A) \leq 0$ , then

$$2\gamma_{\text{f}}(Ax) = \phi''(A) + 8\phi''(2A).$$

Thus, we see that our result reduces precisely to [8, Thm. 4.4] in the case  $y = Ax$  and second neighbour interaction with non-positive  $\phi''(2A)$ . In [8, 6] it was also discussed in depth how such a stability estimate can break down near bifurcation points, even though the atomistic solution is still stable, and that, as a consequence, a bifurcation point may not be correctly predicted.

However, we mention that the above discussion only concerns the stability estimate but not the actual stability of the method. As a matter of fact, numerical evidence is given in [8, Conjecture 1] for stability of the QCF operator as a mapping from  $\mathcal{U}^{1,\infty}$  to  $\mathcal{U}^{-1,\infty}$  up to bifurcation points, and we make similar observations in Section 6.  $\square$

### 4.3 Consistency

In the present section we prove the final ingredient required for the a priori error analysis of the QCF method: the consistency error estimates. We establish these in two separate lemmas in which we treat, respectively, the consistency error for the internal and external forces. We recall from (16) the definition of the modified nodal interpolant  $I_h : \mathcal{V} \rightarrow \mathcal{V}_h$ .

In the following lemma, we use the notation  $\mathcal{L}'_{\text{c}} = \mathcal{L} \setminus \{-\kappa + 1, \dots, \kappa\}$ .



**Lemma 3 (Consistency of Internal Forces)** *Suppose that (13) holds and that  $y \in \mathcal{Y}$ ; then,*

$$\begin{aligned} \|F^{\text{qc}}(I_h y) - f^{\text{a}}(y)\|_{\mathcal{W}_h^{-1,\infty}} &= \sup_{\substack{v_h \in \mathcal{W}_h \\ \|v_h\|_{\mathcal{W}^{1,1}}=1}} \left\{ (F^{\text{qc}}(I_h y), v_h)_h - (f^{\text{a}}(y), v_h)_\varepsilon \right\} \\ &\leq \mathcal{E}_{\text{approx}} + \mathcal{E}_{\text{model}}, \end{aligned}$$

where the approximation error  $\mathcal{E}_{\text{approx}}$  and model error  $\mathcal{E}_{\text{model}}$  are, respectively, given by

$$\mathcal{E}_{\text{approx}} = C_2 \max_{m \in \mathcal{M}_c} h_m^2 \|y''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m-1\})}^2 \quad (50)$$

with the constant  $C_2 = \sup\{\frac{1}{8}|D^3 W(\mathbf{F})| : \mathbf{F} \geq \min_{\xi \in \mathcal{L}'_c} y'_\xi\}$ , and

$$\mathcal{E}_{\text{model}} = 2\varepsilon^2 \max_{\xi \in \mathcal{L}'_c} \sum_{s=\pm 1}^{\pm(r_{\text{cut}}-1)} \left\{ K_{\xi,s}^{(2)} \left| \frac{y'_{\xi+s} - 2y'_\xi + y'_{\xi-s}}{(s\varepsilon)^2} \right| + K_{\xi,s}^{(3)} \left| \frac{y'_{\xi+s} - y'_\xi}{s\varepsilon} \right|^2 \right\}, \quad (51)$$

with decay factors  $K_{\xi,s}^{(j)}$  defined in (30).

*Proof* Let  $(Y_m)_{m \in \mathbb{Z}}$  denote the vector of nodal values of the interpolant  $I_h y$ . Fix  $v_h \in \mathcal{W}_h$  with  $\|v_h\|_{\mathcal{W}^{1,1}} = 1$ ; then, using Proposition 3,

$$\begin{aligned} & - (F^{\text{qc}}(I_h y), v_h)_h + (f^{\text{a}}(y), v_h)_\varepsilon \\ &= \left\{ \sum_{m \in \mathcal{M}_a} \varepsilon \sigma_{\xi_m}^{\text{a}}(I_h y) v'_{h,\xi_m} + \sum_{m \in \mathcal{M}_c} h_m \Sigma_m^c(I_h y) V'_m - \sum_{\xi \in \mathcal{L}} \varepsilon \sigma_\xi^{\text{a}}(y) v'_{h,\xi} \right\} \\ & \quad + \left\{ V_{\bar{K}+1}(\Sigma_{\bar{K}+1}^c - \Sigma_{\bar{K}+1}^{\text{a}}) - V_{\underline{K}-1}(\Sigma_{\underline{K}}^c - \Sigma_{\underline{K}}^{\text{a}}) \right\} =: \text{T}_{\text{bulk}} + \text{T}_{\text{int}}. \end{aligned}$$

First, we focus on the bulk terms. From Assumption (13) it follows that  $I_h y_\xi = y_\xi + C$  for all  $\xi = \zeta + r$ ,  $\zeta \in \mathcal{L}_a$  and  $r = \pm 1, \dots, \pm r_{\text{cut}}$ . This implies that

$$\sigma_{\xi_m}^{\text{a}}(I_h y) = \sigma_{\xi_m}^{\text{a}}(y) \quad \text{for all } m \in \mathcal{M}_a, \quad (52)$$

and hence,  $\text{T}_{\text{bulk}}$  reduces to

$$\begin{aligned} \text{T}_{\text{bulk}} &= \sum_{m \in \mathcal{M}_c} \left\{ h_m \Sigma_m^c(I_h y) V'_m - \sum_{\xi=\xi_{m-1}+1}^{\xi_m} \varepsilon \sigma_\xi^{\text{a}}(y) v'_{h,\xi} \right\} \\ &= \sum_{m \in \mathcal{M}_c} \varepsilon \sum_{\xi=\xi_{m-1}+1}^{\xi_m} (DW(Y'_m) - DW(y'_\xi)) V'_m \\ & \quad + \sum_{m \in \mathcal{M}_c} \varepsilon \sum_{\xi=\xi_{m-1}+1}^{\xi_m} (DW(y'_\xi) - \sigma_\xi^{\text{a}}(y)) V'_m =: \text{T}_{\text{bulk}}^{(1)} + \text{T}_{\text{bulk}}^{(2)}, \end{aligned} \quad (53)$$

where the second equality follows from the fact that  $v'_{h,\xi} = V'_m$  and  $I_h y'_\xi = Y'_m$  for  $\xi = \xi_{m-1} + 1, \dots, \xi_m$ .

Using the model error estimate from Theorem 1 to estimate the difference  $DW(y'_\xi) - \sigma_\xi^a(y)$ , we obtain

$$\begin{aligned}
T_{\text{bulk}}^{(2)} &\leq \sum_{m \in \mathcal{M}_c} \varepsilon \sum_{\xi=\xi_{m-1}+1}^{\xi_m} |DW(y'_\xi) - \sigma_\xi^a(y)| |v'_{h,\xi}| \\
&\leq \|v_h\|_{\mathcal{W}^{1,1}} \max_{m \in \mathcal{M}_c} \max_{\xi=\xi_{m-1}, \dots, \xi_m} \varepsilon^2 \sum_{s=\pm 1}^{\pm(r_{\text{cut}}-1)} \left\{ K_{\xi,s}^{(2)} \left| \frac{y'_{\xi+s} - 2y'_\xi + y'_{\xi-s}}{(s\varepsilon)^2} \right| \right. \\
&\quad \left. + K_{\xi,s}^{(3)} \left| \frac{y'_{\xi+s} - y'_\xi}{s\varepsilon} \right|^2 \right\} \\
&\leq \frac{1}{2} \mathcal{E}_{\text{model}} \|v_h\|_{\mathcal{W}^{1,1}}, \tag{54}
\end{aligned}$$

where the decay factors  $K_{\xi,s}^{(j)}$  are defined in (30).

To estimate the difference  $DW(Y'_m) - DW(y'_\xi)$  appearing in  $T_{\text{bulk}}^{(1)}$  we use the following expansion:

$$DW(y'_\xi) - DW(Y'_m) = D^2W(Y'_m)(y'_\xi - I_h y'_\xi) + \frac{1}{2} D^3W(\theta_\xi)(y'_\xi - I_h y'_\xi)^2,$$

where  $\theta_\xi \in \text{conv}\{Y'_m, y'_\xi\}$ . Inserting this expansion into the first group in (53) we can estimate

$$\begin{aligned}
&\left| \varepsilon \sum_{\xi=\xi_{m-1}+1}^{\xi_m} (DW(I_h y'_\xi) - DW(y'_\xi)) \right| \\
&\leq \left| \varepsilon \sum_{\xi=\xi_{m-1}+1}^{\xi_m} D^2W(Y'_m)(y'_\xi - I_h y'_\xi) \right| + \frac{1}{2} \varepsilon \sum_{\xi=\xi_{m-1}+1}^{\xi_m} |D^3W(\theta_\xi)| |y'_\xi - I_h y'_\xi|^2.
\end{aligned}$$

Since  $I_h y_{\xi_n} = y_{\xi_n} + C$  for all  $n$ , and since  $D^2W(Y'_m)$  is simply a constant in this sum, it follows that the first term on the right-hand side of the inequality vanishes, and we obtain

$$T_{\text{bulk}}^{(1)} \leq 4C_2 \|y - I_h y\|_{\mathcal{W}^{1,\infty}}^2 \|v_h\|_{\mathcal{W}^{1,1}}.$$

Using the interpolation error estimate (17) we finally arrive at

$$\begin{aligned}
T_{\text{bulk}}^{(1)} &\leq 4C_2 \max_{m \in \mathcal{M}_c} \left( \frac{1}{2} h_m \|y''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m-1\})} \right)^2 \|v_h\|_{\mathcal{W}^{1,1}} \\
&= \mathcal{E}_{\text{approx}} \|v_h\|_{\mathcal{W}^{1,1}}. \tag{55}
\end{aligned}$$

To estimate the interface terms, we use Lemma 4 and Theorem 1, to obtain

$$T_{\text{int}} \leq \max_{m=\underline{K}, \overline{K}+1} |\Sigma_m^c - \Sigma_m^a| (|V_{\underline{K}-1}| + |V_{\overline{K}+1}|) \leq \frac{1}{2} \mathcal{E}_{\text{model}} \|v_h\|_{\mathcal{W}^{1,1}}. \tag{56}$$

Combining (54), (55), and (56) gives the stated result.  $\square$

*Remark 7* We note that both the model error  $\mathcal{E}_{\text{model}}$  and the approximation error  $\mathcal{E}_{\text{approx}}$  are formally of second order, despite the fact that the approximation space consists only of piecewise linear polynomials. The proof of this fact for  $\mathcal{E}_{\text{approx}}$  is related to the well-known fact that, in one dimension, the finite element approximation of an linear elliptic problem coincides with the interpolant of the exact solution; see, e.g., [3].

The occurrence of this superconvergence effect also depends crucially on the assumption (13). Without it we would have been unable to assume that  $\sigma_{\xi_m}^a(I_h y) = \sigma_{\xi_m}^a(y)$  for  $m \in \mathcal{M}_a$  (see (52)) and would have obtained additional  $O(\varepsilon)$  terms in the approximation error estimate.  $\square$

**Lemma 4** *We have  $\|v_h\|_{\ell^\infty} \leq \frac{1}{2}\|v'_h\|_{\ell^1_\varepsilon}$  for all  $v_h \in \mathcal{U}_h$ .*

*Proof* This result follows from [26, Lemma A.2].  $\square$

Our final lemma in this section estimates the error committed by approximating the inner product  $(g, v_h)_\varepsilon$  by  $(g, v_h)_h$  in the external forcing term. The following result follows immediately from the estimates in [26] (see in particular Equation (20) and the estimates at the end of Section 3.4).

**Lemma 5 (Consistency of External Forces)** *The consistency error for the external forces is bounded as follows:*

$$\|(g, \cdot)_\varepsilon - (g, \cdot)_h\|_{\mathcal{U}_h^{-1, \infty}} := \sup_{\substack{v_h \in \mathcal{U}_h \\ \|v_h\|_{\mathcal{U}_h^{1, 1}} = 1}} |(g, v_h)_\varepsilon - (g, v_h)_h| \leq \mathcal{E}_{\text{ext}},$$

where

$$\begin{aligned} \mathcal{E}_{\text{ext}} := & \max_{m \in \mathcal{M}_c} h_m^2 \max \left\{ \|g''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m-1\})}, \right. \\ & \left. 2\|g'\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m-1\})} + 2\|g'\|_{\ell^\infty(\{\xi_{m-1}+2, \dots, \xi_m\})} \right\}. \end{aligned} \quad (57)$$

#### 4.4 A priori error estimate

Combining the technical tools assembled in Section 4.1, 4.2, and 4.3, it is now a relatively straightforward matter to establish an existence result and an a priori error estimate.

Let us first recall the main ingredients: In the consistency analysis of Section 4.3 we can identify three sources of the consistency error: the model error  $\mathcal{E}_{\text{model}}$ , the approximation error  $\mathcal{E}_{\text{approx}}$ , and the error due to approximation of the external forces  $\mathcal{E}_{\text{ext}}$ , which are, respectively, defined in (51), (50), and (57). We also recall the definition of the QCF stability constant  $\gamma_f(y_h)$  in (38), which we extend to all  $y \in \mathcal{Y}$  using the same formula.

The following theorem should be read as follows: *If  $y^a$  is a “sufficiently stable” solution of the atomistic model (3), and if  $y^a$  and  $g$  are “sufficiently smooth” in the continuum region, then there exists a solution  $y_h^{\text{qc}}$  of the QCF approximation (11), with quasi-optimal error estimates for  $y^a - y_h^{\text{qc}}$ .*

**Theorem 3** Let  $y^a \in \mathcal{Y}$  be a critical point of the atomistic energy  $\Phi_{\text{tot}}^a$ , that is, it satisfies (7), and suppose that  $\gamma_f(y^a) > 0$ . In addition, suppose that (13) holds.

Under these conditions there exists a constant  $\delta > 0$ , which depends only on  $\min(y^a)'$  and on  $\gamma_f(y^a)$ , such that, if

$$\mathcal{E}_{\text{model}} + \mathcal{E}_{\text{approx}} + \mathcal{E}_{\text{ext}} < \delta, \quad (58)$$

then there exists a locally unique solution  $y_h^{\text{qc}} \in \mathcal{Y}_h$  of the QCF system (11) satisfying

$$\begin{aligned} \|y_h^{\text{qc}} - y^a\|_{\mathcal{W}^{1,\infty}} &\leq \max_{m \in \mathcal{M}_c} \frac{1}{2} h_m \|(y^a)''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m-1\})} \\ &\quad + 4\gamma_f(y^a)^{-1} (\mathcal{E}_{\text{model}} + \mathcal{E}_{\text{approx}} + \mathcal{E}_{\text{ext}}). \end{aligned} \quad (59)$$

Moreover, we have the superconvergence result

$$\|y_h^{\text{qc}} - I_h y^a\|_{\mathcal{W}^{1,\infty}} \leq 4\gamma_f(y^a)^{-1} (\mathcal{E}_{\text{model}} + \mathcal{E}_{\text{approx}} + \mathcal{E}_{\text{ext}}). \quad (60)$$

*Remark 8* 1. We call estimate (60) a superconvergence result since all terms on the right-hand side are formally of second order.

2. Upon investigating the proof of the inverse function theorem, Lemma 6, it becomes clear that the factor 4 in (59) and (60) may be replaced by any constant that is strictly greater than 1, at the cost of a smaller constant  $\delta$  in (58).

3. By far the most stringent condition, and the only condition we consider potentially problematic, is the stability assumption  $\gamma_f(y^a) > 0$ , which we have discussed in detail in Remark 6.  $\square$

Before we give the proof of the theorem, we need to state two more auxiliary results. The principle underlying the existence proof is the following explicit variant of the inverse function theorem, which is inspired by [29, Section 3].

**Lemma 6 ([25], Lemma 1)** Let  $\hat{X}, \hat{Y}$  be Banach spaces,  $\hat{A}$  an open subset of  $\hat{X}$ , and let  $\hat{F} : \hat{A} \rightarrow \hat{Y}$  be Fréchet differentiable. Suppose that  $\hat{x}_0 \in \hat{A}$  satisfies the conditions

$$\|\hat{F}(\hat{x}_0)\|_{\hat{Y}} \leq \eta, \quad (61)$$

$$\|D\hat{F}(\hat{x}_0)^{-1}\|_{L(\hat{Y}, \hat{X})} \leq \sigma, \quad (62)$$

$$\overline{B_{\hat{X}}(\hat{x}_0, 2\eta\sigma)} \subset \hat{A}, \quad (63)$$

$$\|D\hat{F}(\hat{x}_1) - D\hat{F}(\hat{x}_2)\|_{L(\hat{X}, \hat{Y})} \leq L\|\hat{x}_1 - \hat{x}_2\|_{\hat{X}} \quad \text{for } \|\hat{x}_j - \hat{x}_0\|_{\hat{X}} \leq 2\eta\sigma, \quad (64)$$

$$j = 1, 2,$$

$$\text{and } 2L\sigma^2\eta < 1; \quad (65)$$

then, there exists a locally unique  $\hat{x} \in \hat{X}$  such that  $\hat{F}(\hat{x}) = 0$  and  $\|\hat{x} - \hat{x}_0\|_{\hat{X}} \leq 2\eta\sigma$ .

Motivated by the previous result, we also establish local Lipschitz continuity of  $DF^{\text{qc}}$  and, as a consequence, Fréchet differentiability of  $F^{\text{qc}}$  in  $\mathcal{Y}_h$ . The proof is a simple calculus exercise and is therefore omitted.

**Lemma 7** *The operator  $F^{\text{qc}}$  is Fréchet differentiable in  $\mathcal{Y}$ , and, for each  $\mu > 0$  there exists a constant  $L = L(\mu)$  such that, for all  $y_h, \bar{y}_h \in \mathcal{Y}_h$  with  $\min y'_h \geq \mu$  and  $\min \bar{y}'_h \geq \mu$ , we have the Lipschitz condition*

$$\begin{aligned} ((DF^{\text{qc}}(y_h) - DF^{\text{qc}}(\bar{y}_h))u_h, v_h)_h &\leq L \|y_h - \bar{y}_h\|_{\mathcal{U}^{1,\infty}} \|u_h\|_{\mathcal{U}^{1,\infty}} \|v_h\|_{\mathcal{U}^{1,1}} \\ &\text{for all } u_h, v_h \in \mathcal{U}_h. \end{aligned}$$

*Proof (Proof of Theorem 3)* For the sake of brevity, we set  $y = y^{\text{a}}$  throughout this proof. The argument is a straightforward application of the inverse function theorem. In the notation of Lemma 6 we set  $\hat{X} = \mathcal{U}_h^{1,\infty}$ ,  $\hat{Y} = \mathcal{U}_h^{-1,\infty}$ ,  $\hat{x}_0 = 0$ ,  $\hat{F}(u_h) = -(F^{\text{qc}}(I_h y + u_h) + g, \cdot)_h$ , and  $\hat{A} = B_{\hat{X}}(0, \frac{1}{2} \min y')$  so that

$$\min(I_h y' + u'_h) \geq \frac{1}{2} \min y' \quad \text{for all } u_h \in \hat{A}.$$

Lemmas 3 and 5 give the following residual estimate

$$\begin{aligned} \|\hat{F}(0)\|_{\hat{Y}} &\leq \|F^{\text{qc}}(I_h y) - f^{\text{a}}(y)\|_{\mathcal{U}_h^{-1,\infty}} + \|(g, \cdot)_h - (g, \cdot)_\varepsilon\|_{\mathcal{U}_h^{-1,\infty}} \\ &\leq \mathcal{E}_{\text{model}} + \mathcal{E}_{\text{approx}} + \mathcal{E}_{\text{ext}} =: \eta, \end{aligned}$$

which establishes (61).

Next, we note that

$$\min_{\xi=\xi_{m-1}+1, \dots, \xi_m} \mu_\xi^{\text{qc}}(I_h y) = Y'_m \geq \min_{\xi=\xi_{m-1}+1, \dots, \xi_m} \mu_\xi^{\text{qc}}(y) \quad \text{for all } m \in \mathcal{M}_c.$$

Moreover, using the interpolation error estimate (17), we have

$$|\phi''(I_h y'_\xi) - \phi''(y'_\xi)| \leq C_3 \frac{1}{2} h_m \|y''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m\})},$$

where  $C_3 = \overline{\phi}'''(\min_{\xi \in \mathcal{L}'_c} y'_\xi)$ , and hence we obtain from the definition of  $\gamma_f$  in (38) that

$$\gamma_f(I_h y) \geq \gamma_f(y) - C_3 \frac{1}{2} \max_{m \in \mathcal{M}_c} h_m \|y''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m\})}.$$

Thus, if

$$\max_{m \in \mathcal{M}_c} h_m \|y''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m\})} \leq \gamma_f(y)/C_3 =: \delta_1, \quad (66)$$

then (62) holds with  $\sigma = 2/\gamma_f(y)$ . Condition (66) may, equivalently, be written as

$$\mathcal{E}_{\text{approx}} < C_2 \delta_1^2,$$

which will automatically be satisfied if we choose  $\delta \leq C_2 \delta_1^2$  in (58).

To satisfy (63), we require that

$$2\eta\sigma < \mu, \quad \text{or, equivalently,} \quad \eta < \frac{1}{4}\mu\gamma_f.$$

Lemma 7 now gives us a Lipschitz condition  $L = L(\mu)$  required in (64), and we are only left to satisfy the final condition (65), which may be rewritten as

$$\eta < (4L)^{-1}\gamma_f^2.$$

In summary, if

$$\mathcal{E}_{\text{model}} + \mathcal{E}_{\text{approx}} + \mathcal{E}_{\text{ext}} < \min\left(\frac{1}{4}\mu\gamma_f, \frac{1}{4}L^{-1}\gamma_f^2, C_2\delta_1^2\right) =: \delta,$$

then all conditions of Lemma 6 are satisfied, and the existence of a solution  $y_h^{\text{qc}} = \mathbf{A}x + u_h$  as well as the stated estimate (60) follow.

The estimate (59) is an immediate consequence of (60) and the triangle inequality.  $\square$

## 5 Formulation and Analysis of a Stress-Based Coupling Mechanism

### 5.1 Coupling of stresses

The analyses in [8, 9] and our own analysis of the weak form (37) of the QCF method have clearly revealed that the interface terms caused severe technical difficulties and indeed some worrying properties of the QCF method, primarily the lack of positivity of the linearized operator ([9, Thm. 1] and [8, Thm. 4.1]) and the lack of  $\varepsilon$ -uniform stability in any  $\mathcal{U}^{1,p}$ -norm,  $1 \leq p < \infty$  ([9, Thm. 4] and [8, Thm. 4.3]). Therefore, we seek to formulate a new coupling mechanism that overcomes these deficiencies, but retains the high accuracy of the QCF method.

To motivate the new method we remark that, while forces are natural objects in atomistic simulation, the stress (and hence the weak form (21)) is a much more natural concept in continuum mechanics. Thus, it is a natural idea to couple the two weak forms of the equilibrium equations (21) and (24), which leads to the stress-based atomistic/continuum (SAC) method

$$\text{Find } y_h^{\text{ac}} \in \mathcal{Y}_h \text{ s.t. } \langle S^{\text{ac}}(y_h^{\text{ac}}), v_h \rangle = (g, v_h)_h \quad \forall v_h \in \mathcal{U}_h, \quad (67)$$

where  $S^{\text{ac}} : \mathcal{Y}_h \rightarrow \mathcal{U}_h^*$  is defined by

$$\langle S^{\text{ac}}(y_h), v_h \rangle = \sum_{m \in \mathcal{M}_a} \varepsilon V'_m \Sigma_m^a(y_h) + \sum_{m \in \mathcal{M}_c} h_m V'_m \Sigma_m^c(y_h). \quad (68)$$

Here we have used the notation  $\Sigma_m^c$  defined in (21),  $\Sigma_m^a$  in (36), and  $\mathcal{M}_a$  and  $\mathcal{M}_c$  in (35).

An alternative motivation for the definition of the operator  $S^{\text{ac}}$  is that it can be obtained from the weak form of the QCF method (37) by dropping the atomistic/continuum interface terms, thus weakly imposing equality of normal stresses at the interface between the two models.

It turns out that the techniques we have developed in Sections 3 and 4 for the analysis of the QCF method are sufficient for the analysis of this new scheme, and indeed lead to stronger results.

## 5.2 A priori error estimates

We begin by establishing a stability result in  $\mathcal{W}^{1,\infty}$ . For the following results we redefine the set  $\mathcal{L}'_c$  as  $\mathcal{L}'_c = \mathcal{L} \setminus \{-\kappa, \dots, \kappa + 1\}$ .

**Lemma 8 (Stability)** *Let  $y_h \in \mathcal{Y}_h$ ; then,*

$$\inf_{\substack{u_h \in \mathcal{U}_h \\ \|u_h\|_{\mathcal{W}^{1,\infty}}=1}} \sup_{\substack{v_h \in \mathcal{U}_h \\ \|v_h\|_{\mathcal{W}^{1,1}}=1}} \langle DS^{\text{ac}}(y_h)u_h, v_h \rangle \geq \gamma_s(y_h), \quad \text{where}$$

$$\gamma_s(y_h) = \frac{1}{2} \min \left\{ \min_{\xi \in \mathcal{L}'_c} D^2W(y'_{h,\xi}), \min_{\xi \in \mathcal{L} \setminus \mathcal{L}'_c} \left( \phi''(y'_{h,\xi}) - \sum_{r=2}^{r_{\text{cut}}} r^2 \overline{\phi''}(r\mu_\xi^a(y_h)) \right) \right\}.$$

*Proof* It is easy to see that  $S^{\text{ac}}$  is differentiable in  $\mathcal{Y}_h$ . Defining  $(\mathcal{J}_{m,n})_{m,n=1}^M$  as

$$\mathcal{J}_{m,n} = \begin{cases} \mathcal{H}_{mn}^a, & m \in \mathcal{M}_a, \\ \mathcal{H}_{mn}^c, & m \in \mathcal{M}_c, \end{cases}$$

we obtain

$$\langle DS^{\text{ac}}(y_h)u_h, v_h \rangle = \sum_{m,n=1}^M h_m \mathcal{J}_{mn} V'_m U'_n.$$

The result follows by applying Lemma 1 and using (42).  $\square$

*Remark 9* We note that this stability result is valid in a larger region of deformations than Theorem 2. To see this we show that, under reasonable assumptions on the interaction potential, the estimate is sharp when evaluated at a homogeneous deformation.

If we insert the homogeneous deformation  $y = Ax$ , and assume that

$$-\overline{\phi''}(rA) = \phi''(rA) \quad \text{for } r \geq 2$$

(e.g., if  $\phi$  is a Lennard–Jones or Morse potential), then we obtain

$$\gamma_s(Ax) = \frac{1}{2} \min \left( D^2W(A), \phi''(A) + \sum_{r=2}^{r_{\text{cut}}} r^2 \phi''(rA) \right) = \frac{1}{2} D^2W(A).$$

Hence, we have shown that  $DS^{\text{ac}}(Ax)$  is stable up to the critical strain  $A$  at which  $D^2\Phi_c(Ax)$  becomes unstable.  $\square$

The next lemma is a counterpart of the consistency error estimate, Lemma 3. Its proof is obtained by simply ignoring the interface terms in the proof of Lemma 3. The consistency error estimate for the external forces, Lemma 5, can be used without changes.

**Lemma 9 (Consistency)** *Let  $y \in \mathcal{Y}$ , and suppose that (13) holds; then,*

$$\|S^{\text{ac}}(I_h y) + f^{\text{a}}(y)\|_{\mathcal{U}_h^{-1,\infty}} \leq \mathcal{E}_{\text{approx}}^{\text{s}}(y) + \mathcal{E}_{\text{model}}^{\text{s}}(y) + \mathcal{E}_{\text{ext}},$$

where the approximation error  $\mathcal{E}_{\text{approx}}^{\text{s}}$  is given by

$$\mathcal{E}_{\text{approx}}^{\text{s}} = C_3 \max_{m \in \mathcal{M}_c} h_m^2 \|y''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m-1\})}, \quad (69)$$

with constant  $C_3 = \sup\{\frac{1}{8}|D^3 W(F)| : F \geq \min_{\xi \in \mathcal{L}'_c} y'_\xi\}$ , and the model error  $\mathcal{E}_{\text{model}}^{\text{s}}$  is given by

$$\mathcal{E}_{\text{model}}^{\text{s}}(y) = \varepsilon^2 \max_{\xi \in \mathcal{L}'_c} \sum_{r=\pm 2}^{\pm(r_{\text{cut}}-1)} \left\{ K_{\xi,s}^{(2)} \left| \frac{y'_{\xi+s} - 2y'_\xi + y'_{\xi-s}}{(s\varepsilon)^2} \right| + K_{\xi,s}^{(3)} \left| \frac{y'_{\xi+s} - y'_\xi}{s\varepsilon} \right|^2 \right\}, \quad (70)$$

with decay factors  $K_{\xi,s}^{(j)}$  defined in (30).

Finally, we formulate a counterpart of Lemma 7, again without proof.

**Lemma 10** *The operator  $S^{\text{ac}}$  is Fréchet differentiable in  $\mathcal{Y}_h$  and, for each  $\mu > 0$  there exists a constant  $L = L(\mu)$  such that, for all  $y_h, \bar{y}_h \in \mathcal{Y}_h$  with  $\min y'_h \geq \mu$  and  $\min \bar{y}'_h \geq \mu$ , we have the Lipschitz condition*

$$\langle (DS^{\text{ac}}(y_h) - DS^{\text{ac}}(\bar{y}_h))u_h, v_h \rangle \leq L \|y_h - \bar{y}_h\|_{\mathcal{U}^{1,\infty}} \|u_h\|_{\mathcal{U}^{1,\infty}} \|v_h\|_{\mathcal{U}^{1,1}} \\ \forall u_h, v_h \in \mathcal{U}_h.$$

Thus, we have all ingredients in place to establish the counterpart of the a priori existence result and error estimate of Theorem 3. The proof of the following theorem can be obtained by repeating the proof of Theorem 3 verbatim.

**Theorem 4** *Let  $y^{\text{a}} \in \mathcal{Y}$  be a critical point of the atomistic energy  $\Phi_{\text{tot}}^{\text{a}}$ , that is, it satisfies (7), and suppose that  $\gamma_{\text{s}}(y^{\text{a}}) > 0$ . In addition, suppose that (13) holds.*

*Under these conditions there exists a constant  $\delta > 0$ , which depends only on  $\min(y^{\text{a}})'$  and on  $\gamma_{\text{s}}(y)$ , such that, if*

$$\mathcal{E}_{\text{model}}^{\text{s}}(y^{\text{a}}) + \mathcal{E}_{\text{approx}}^{\text{s}}(y^{\text{a}}) + \mathcal{E}_{\text{ext}} < \delta, \quad (71)$$

then there exists a locally unique solution  $y_h^{\text{ac}} \in \mathcal{Y}_h$  of the stress coupling method (67) satisfying

$$\|y_h^{\text{ac}} - y^{\text{a}}\|_{\mathcal{U}^{1,\infty}} \leq \max_{m \in \mathcal{M}_c} \frac{1}{2} h_m \|(y^{\text{a}})''\|_{\ell^\infty(\{\xi_{m-1}+1, \dots, \xi_m-1\})} \\ + 4\gamma_{\text{s}}(y^{\text{a}})^{-1} (\mathcal{E}_{\text{model}}^{\text{s}}(y^{\text{a}}) + \mathcal{E}_{\text{approx}}^{\text{s}}(y^{\text{a}}) + \mathcal{E}_{\text{ext}}). \quad (72)$$

Moreover, we have the superconvergence result

$$\|y_h^{\text{ac}} - I_h y^{\text{a}}\|_{\mathcal{U}^{1,\infty}} \leq 4\gamma_{\text{s}}(y^{\text{a}})^{-1} (\mathcal{E}_{\text{model}}^{\text{s}}(y^{\text{a}}) + \mathcal{E}_{\text{approx}}^{\text{s}}(y^{\text{a}}) + \mathcal{E}_{\text{ext}}). \quad (73)$$



*Remark 10* Although Theorem 4 may appear, at a first glance, no different from Theorem 3, the conditions of Theorem 4 are in fact significantly weaker. This is primarily due to a much sharper stability result, which can be expected to hold up to bifurcation points (see Remark 9). A rigorous investigation of this statement for large deformations is still open.  $\square$

*Remark 11* It turns out that, unlike the linearized QCF operator, the linearized SAC operator is positive definite, except possibly close to bifurcation points. This fact is established in [20]. As a consequence, it follows that under suitable assumptions on  $y$ ,  $DS^{\text{ac}}(I_h y)$  is stable in  $\mathcal{W}_h^{1,2}$  and in fact, using the Riesz–Thorin interpolation theorem, in  $\mathcal{W}_h^{1,p}$  for  $2 \leq p \leq \infty$ . It is easy to generalize the consistency result of Lemma 9 to give consistency error estimates in  $\mathcal{W}_h^{-1,p}$  and we can therefore obtain quasi-optimal error estimates for the SAC method in  $\mathcal{W}_h^{1,p}$  for  $2 \leq p \leq \infty$ .

Moreover, the fact that  $DS^{\text{ac}}$  is positive definite makes a generalization of the a priori error analysis to two and three dimensions feasible. Note that  $\mathcal{W}_h^{1,\infty}$ -stability results cannot be expected to hold in more than one dimension.  $\square$

## 6 Numerical Experiments

Our implementations of the QCF and SAC methods assume second-neighbour interactions ( $r_{\text{cut}} = 2$ ), where the interaction potential is a Morse potential  $\phi(r) = e^{-2\alpha(r-1)} - 2e^{-\alpha(r-1)}$  with  $\alpha = 3$ . The results of the numerical experiments do not change qualitatively for different values of  $\alpha$ .

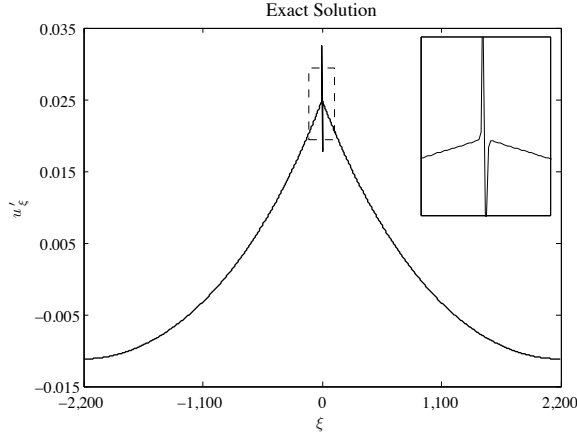
In all experiments we set  $N = 2200$  and let the external force be defined by

$$g_\xi = \begin{cases} -1 - x_\xi, & \xi = -N + 1, \dots, -2, \\ -\frac{1}{10}N, & \xi = -1, \\ \frac{1}{5}N, & \xi = 0, \\ -\frac{1}{10}C_2N, & \xi = 1, \\ 1 - x_\xi, & \xi = 1, \dots, N. \end{cases} \quad (74)$$

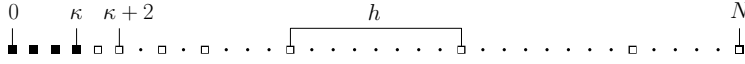
This forcing function was chosen so that the curvature of the solution has roughly the same order of magnitude throughout the domain, which allows us to observe the predicted convergence rates. The large oscillations of the force at  $\xi = -1, 0, 1$  cause the solution to be highly non-smooth at the origin, which has a similar effect as a defect. The exact atomistic solution with  $A = 1$  is displayed in Figure 2.

Given a maximal meshsize  $h$  and an atomistic region  $\{-\kappa, \dots, \kappa\}$ , we construct the set  $\mathcal{L}_{\text{rep}} = \mathcal{L}_{\text{rep}}(\kappa, h)$  as follows:

1. We add the indices  $0, \pm 1, \dots, \pm(\kappa + 2)$  to  $\mathcal{L}_{\text{rep}}$ .
2. We add the indices  $\pm(\kappa + 2 + 2^j)$ ,  $j = 1, \dots, J$ , to  $\mathcal{L}_{\text{rep}}(\kappa, h)$ , where  $J$  is chosen maximally so that no element diameter exceeds  $h$ .



**Fig. 2** Atomistic solution with  $r_{\text{cut}} = 2$ ,  $N = 2200$ , interaction potential  $\phi(r) = e^{-2\alpha(r-1)} - 2e^{-\alpha(r-1)}$  with  $\alpha = 3$ , macroscopic strain  $A = 1$ , and external force  $g$  defined by (74).



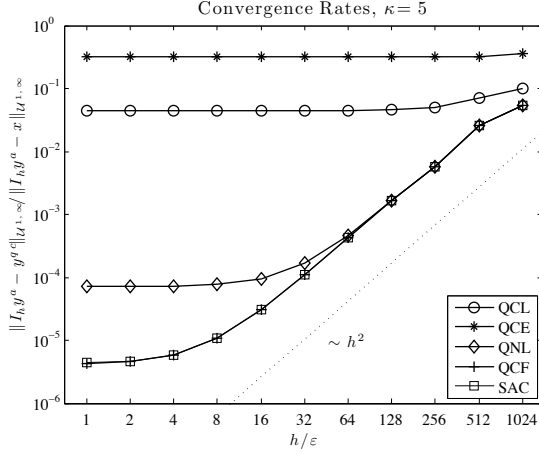
**Fig. 3** Visualisation of the construction of  $\mathcal{L}_{\text{rep}}(\kappa, h)$  with parameters  $\kappa = 3$ ,  $r_{\text{cut}} = 2$ ,  $N = 34$ , and  $h = 8\varepsilon$ .

3. We add the indices  $\kappa + 2 + 2^J + k2^{J-1}$  to  $\mathcal{L}_{\text{rep}}(\kappa, h)$ , resulting in a uniform mesh up to the boundary.
4. We add  $N$  to  $\mathcal{L}_{\text{rep}}(\kappa, h)$ , which simplifies the datastructures.

A visualisation of this construction is provided in Figure 3, with parameters  $\kappa = 3$ ,  $r_{\text{cut}} = 2$ ,  $N = 34$ , and  $h = 8\varepsilon$ .

Apart from the QCF and SAC methods we also implemented the full atomistic model to obtain exact comparison solutions, the QCL method (Section 2.4), the original energy-based QC (QCE) method [24] and a flavour of the quasinonlocal QC (QNL) method [32], which is an energy-based QC method without ghost forces. A complete description of these methods would exceed the scope of this paper and we refer instead to [5, 6, 24, 32] for details. An error analysis similar to our present work for the QCL, QCE and QNL methods is given in [27].

To compute local minimizers of the atomistic model we used a nonlinear conjugate gradient method preconditioned by a discrete Laplacian. To compute solutions of the nonlinear systems arising from the various QC formulations we used a truncated Newton method, taking the interpolant of the atomistic solution as the starting guess.



**Fig. 4** Relative error of various atomistic/continuum methods for the model problem described in the beginning of Section 6, with  $A = 1$ ,  $\kappa = 5$ , and varying  $h$ .

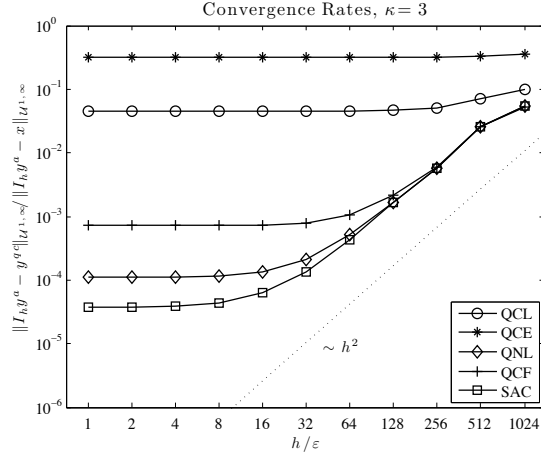
### 6.1 Test 1: a deep equilibrium

In our first numerical test we study the decay of the error as  $h$  approaches  $\varepsilon$ . In Figure 4 we plot the relative errors of displacements, measured in the superconvergent norm

$$\frac{\|I_h y^a - y^{qc}\|_{\mathcal{U}^{1,\infty}}}{\|I_h y^a - Ax\|_{\mathcal{U}^{1,\infty}}},$$

for  $A = 1$ ,  $\kappa = 5$  and varying  $h$ . We observe precisely the predicted  $O(h^2)$  rates of decay for the error of the QCF and SAC methods. As the atomistic spacing is approached we see that the error curve becomes flat, which indicates that the modelling error dominates the discretization error. The QNL method (which has no ghost force) also achieves very good accuracy, however, the first-order interface error observed in [5, 25, 27] becomes dominant well before the second-order modelling error. The error of the QCL method is of course dominated by the “defect”. It is also very interesting to note that, in this particular problem, the error in the QCE method due to the ghost force [5, 23, 31] is even larger than the error committed by the QCL method due to describing the “defect” with the continuum model.

Repeating the test with  $\kappa = 3$ , which is shown in Figure 5, gives rise to an interesting observation. As expected, the errors of the QNL, QCF as well as the SAC method increase due to a smaller atomistic region. It is, however, somewhat unexpected that the QCF method deteriorates far more than the SAC method and becomes even less accurate than the QNL method. We have made similar observations for modified experiments, and hence this indicates that the QCF method may have some difficulties with very small atomistic regions. At this point we are unable to offer an explanation for this effect.



**Fig. 5** Relative error of various atomistic/continuum methods for the model problem described in the beginning of Section 6, with  $A = 1$ ,  $\kappa = 3$ , and varying  $h$ .

## 6.2 Test 2: accuracy near a bifurcation point

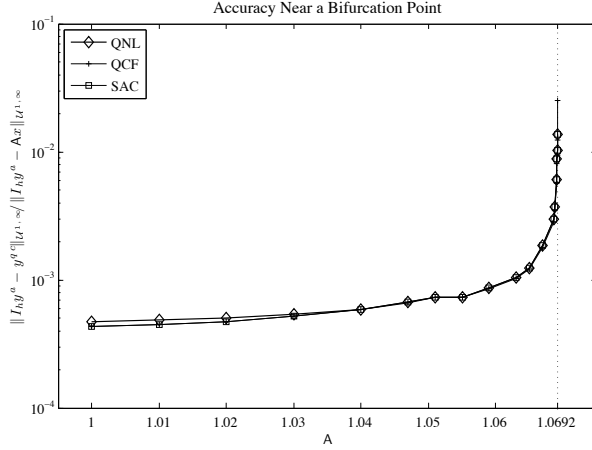
In our second test we investigate the accuracy of the QCF, SAC, and QNL methods as the deformation approaches a bifurcation point. To that end we first compute atomistic solutions with varying macroscopic strain  $A$ . We increase  $A$  in small steps until a critical value  $A_a^{\text{crit}}$  is reached at which the atomistic solution ceases to be stable. Next, for various values of  $A \in [1, A_a^{\text{crit}}]$ , approaching  $A_a^{\text{crit}}$ , we solve the QCF, SAC, and QNL equilibrium equations taking the interpolant of the atomistic solution as the starting guess of the truncated Newton method. If the method fails or does not converge within fifty steps, then we declare the method unstable. Throughout these experiments we choose  $\kappa = 5$ ,  $h = 2^6 \varepsilon$ , for which QCF, SAC and QNL have comparable accuracy in our first test.

The result of this experiment is displayed in Figure 6. We observe that all three methods are stable to within a small distance to the bifurcation point and maintain excellent and comparable accuracy. A finer investigation shows that the critical strains at which QCF, SAC and QNL become unstable exhibit the following relative errors:

$$\frac{|A_a^{\text{crit}} - A_a^{\text{crit}}|}{|A_a^{\text{crit}} - 1|} \approx 2.89 \times 10^{-4}, \quad \frac{|A_a^{\text{crit}} - A_a^{\text{crit}}|}{|A_a^{\text{crit}} - 1|} \approx 4.34 \times 10^{-4},$$

$$\text{and} \quad \frac{|A_a^{\text{crit}} - A_a^{\text{crit}}|}{|A_a^{\text{crit}} - 1|} \approx 4.34 \times 10^{-4}.$$

All relative errors are below  $(2N)^{-1}$ , which is the best order of magnitude of the error that can be expected. We note in particular that the QCF method is stable almost up to the bifurcation point, which we were unable to prove in this paper.



**Fig. 6** Relative error of various atomistic/continuum methods for the model problem described in the beginning of Section 6, with  $h = 2^6 \varepsilon$ ,  $\kappa = 5$ , and varying  $A$  so that the solution approaches a bifurcation point as  $A$  approaches the critical value  $A_a^{\text{crit}} \approx 1.0692$ .

## 7 Conclusion

We have developed an a priori error analysis for two force-based atomistic/continuum hybrid methods: the force-based quasicontinuum (QCF) method and a new stress-based atomistic/continuum (SAC) coupling scheme. Our analysis of the QCF method, and our subsequent formulation of the SAC method were based on a new notion of atomistic stress function, which arises in a convenient weak form of the atomistic equilibrium equations. For example, we described the model error of the Cauchy–Born approximation directly via an error estimate on the Cauchy–Born stress function. This estimate directly enters into the error analysis of the QCF and SAC methods. The formulation and analysis of the atomistic stress function for more general interaction potentials in 1D is straightforward. However, the extension to 2D/3D is an interesting challenge, since there is no unique way of defining the stress function in 2D/3D.

The most challenging aspect of our analysis was the proof of the stability estimate for the QCF method. As in previous works on the QCF method [7–9] we were only able to prove stability in a discrete  $W^{1,\infty}$ -norm. We expect that the formal analogue of such a result in two or three dimensions would be false, which is the main conceptual reason why our analysis is restricted to a one dimensional model problem. Even so, we were unable to prove stability of the QCF method in the entire range of deformations where we observe it in numerical experiments (see remark 6 and [8] for a more detailed discussion of this fact). Thus, a question of crucial importance for the analysis of the QCF method is to find an alternative topology in which stability of the QCF method can be established up to bifurcation points and in two and three dimensions.

By contrast, our stability analysis for the SAC method is valid in the entire region of stability of the atomistic model, up to a controlled error. Moreover, in [20] we showed that the linearization of the SAC method is positive definite (which is not the case for the QCF method) and this makes an analysis of the SAC method in two and three dimensions tractable.

Finally, we remark that even a careful formulation and efficient implementation of the QCF method in two and three dimensions appears to be lacking at this point. Even though the QCF method is the mechanism hidden behind the commonly employed ghost-force correction strategy [4, 31], we expect that one can achieve significant computational gains by solving the QCF system (or possibly the SAC system) directly.

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